#### **SUBTILASES**

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## **CROSS-REFERENCE TO RELATED APPLICATIONS**

This application claims priority or the benefit under 35 U.S.C. 119 of Danish application no. PA 2003 00435 filed March 21, 2003 and U.S. provisional application no. 60/457,798 filed March 26, 2003, the contents of which are fully incorporated herein by reference.

#### FIELD OF THE INVENTION

The present invention relates to JP170 and BPN' like subtilases and to methods of construction such variants with altered properties, such as stability (e.g. thermostability or storage stability), Ca<sup>2+</sup> dependency, pH dependent activity, improved performance in washing and cleaning applications.

#### **BACKGROUND OF THE INVENTION**

Enzymes have been used within the detergent industry as part of washing formulations for more than 30 years. Proteases are from a commercial perspective the most relevant enzyme in such formulations, but other enzymes including lipases, amylases, cellulases or mixtures of enzymes are also often used.

To improve the cost and/or the performance of proteases there is an ongoing search for proteases with altered properties, such as increased activity at low temperatures, increased thermostability, increased specific activity at a given pH, altered Ca<sup>2+</sup> dependency, increased stability in the presence of other detergent ingredients (e.g. bleach, surfactants etc.) etc.

The search for proteases with altered properties include both discovery of naturally occurring proteases, i.e. so called wild-type proteases but also alteration of well-known proteases by e.g. genetic manipulation of the nucleic acid sequence encoding said proteases. Knowledge of the relationship between the three-dimensional structure and the function of a protein has improved the ability to evaluate which areas of a protein to alter to affect a specific characteristic of the protein.

One family of proteases, which are often used in detergents, are the subtilases. This family has previously been further grouped into 6 different sub-groups by Siezen RJ and

Leunissen JAM, 1997, Protein Science, 6, 501-523. One of these sub-groups is the Subtilisin family which includes subtilases such as BPN', subtilisin 309 (SAVINASE®, NO-VOZYMES A/S), subtilisin Carlsberg (ALCALASE®, NOVOZYMES A/S), subtilisin S41 (a subtilase from the psychrophilic Antarctic *Bacillus* TA41, Davail S et al. 1994, The Journal of Biological Chemistry, 269(26), 99. 17448-17453), subtilisin S39 (a subtilase from the psychrophilic Antarctic *Bacillus* TA39, Narinx E et al. 1997, Protein Engineering, 10 (11), pp. 1271-1279) and TY145 (a subtilase from Bacillus sp. TY145, NCIMB 40339 described in WO 92/17577).

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The groupings indicated above were made based on primary sequence alignments, with only little consideration of three-dimensional structure. However, despite sequence homologies between subtilases belonging to the Subtilisin subgroup, modelling of the three-dimensional structure of one subtilase on the basis of the three-dimensional structure of another subtilase (such as the subtilisin BPN' that was used by Siezen and Leunissen) may result in an incorrect three-dimensional model structure because of structural differences.

Recently the three-dimensional structure of subtilase TY145 have been elucidated and it was found that there are several differences between this and the three-dimensional structure of BPN' also belonging to the Subtilisin subgroup of subtilases (PCT/DK2004/000066).

The differences between the three-dimensional structures of TY145 and BPN' are confirmed by the three-dimensional structure of the subtilase "sphericase" from *Bacillus sphaericus* (PDB NO:1EA7, Protein Data Bank). The overall structure and many details of this subtilase are very homologous with the TY145 subtilase structure.

The subtilase JP170 and subtilases similar to JP170 are already known in the art, but the three-dimensional structure has not been disclosed for such subtilases.

The JP170 subtilase was described as protease A in WO 88/01293 to Novozymes. Later the patent application WO 98/56927 to Novozymes Biotech disclosed the amino acid (polypeptide) sequence of JP170 and the DNA sequence encoding JP170. In EP 204 342 the protease Ya was disclosed, and JP7-62152 and JP 4197182 to Lion Corp. disclosed the DNA sequence encoding protease Ya produced by *Bacillus sp.* Y that is homologous to JP170. In addition US 6,376,227 to Kao Corp. discloses physical characteristics as well as DNA and polypeptide sequences of alkaline proteases KP43, KP1790 and KP9860 which are also homologous to JP170. Recently variants of the KP43, KP9860, SD-521 and Ya proteases among others were disclosed in EP 1209233. These proteases are highly ho-

mologous, and an alignment of KP43, KP9860, SD-521, Y and JP170 revealed at least 90% homology. Therefore JP170, Ya and SD-521 represent these proteases in the alignment of Fig. 1 of the present specification.

# 5 BRIEF DESCRIPTION OF THE FIGURES

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Figure 1 shows an alignment of three JP170 type proteases: (a) SD-521 (EP 1 209 233), (b) protease Ya (WO 99/67370), and (c) JP170 (WO 98/56927, mature sequence from Appendix 1).

Figure 2 shows a superposition of the 3D structures of the proteases JP170 and Savinase (BLSAVI), with indication of calcium binding sites. In the figure JP170 is indicated in light grey with three ion-binding sites, and Savinase in a dark structure with two ion-binding sites.

Figure 3 shows a matrix of homology between amino acid sequences of subtilases pertaining to various subtilase subgroups. The sequences are identified by sequence database accession numbers and their derivation.

- 1: aam50084; Subtilase derived from Bacillus sp. strain SD-521
- 2: aaw89547; Subtilase derived from Bacillus sp. JP170
- 3: q45681; Subtilase derived from B. subtilis (BSTA41)
- 4: p28842; Psychrophilic subtilisin derived from Antarctic Bacillus strain (BSTA39)
- 5: abb77095; Subtilase derived from Bacillus sp. (TY145)
  - 6: p00783; Subtilase derived from Bacillus subtilis var. amylosacchariticus (BSAMY)
  - 7: p29142; Subtilase derived from Bacillus stearothermophilus (BSSJ)
  - 8: p35835; Subtilase derived from Bacillus subtilis var. natto. (BSNAT)
  - 9: p07518; Subtilase derived from Bacillus pumilus (B. mesentericus) (BPMES)
- 10: p00782; Subtilase derived from Bacillus amyloliquefaciens (BPN')
  - 11: p00780; Subtilase derived from Bacillus licheniformis (BLSCAR)
  - 12: p41363; Subtilase derived from Bacillus halodurans (BHSAH)
  - 13: aaw62222; Subtilase derived from Bacillus lentus (BLS147)
  - 14: p29600; Subtilase derived from Bacillus lentus (BLSAVI, BLS309)
- 15: p27693; Subtilase derived from *Bacillus alcalophilus* (BAALKP)
  - 16: q99405; Subtilase derived from Bacillus sp. strain KSM-K16 (BSKSMK)
  - 17: p29599; Subtilase derived from Bacillus lentus (BLSUBL).

Sequences 1 and 2 belong to the JP170 type, sequences 3 to 5 belong to the TY145

type, sequences 6 to 11 belong to the "true subtilisins" or I-S1 type, and sequences 12 to 17 belong to the "highly alkaline" subtilisins or I-S2 type. From Fig. 3 it is clear that these types are quite distinct.

Figure 4 shows a three-dimensional alignment of the subtilases:

(1) Ty145; (2) BPN'; (3) Savinase; and (4) JP170.

By 3D sequences is meant that the position of homologous residues are chosen by superposition of the 3D structures and subsequently the amino acid sequences are aligned based on these homologous positions.

## BRIEF DESCRIPTION OF THE APPENDIX

APPENDIX 1 shows the structural coordinates for the solved crystal structure of JP170.

#### **SEQUENCE LISTING**

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In the appended sequence listing the following amino acid sequences are provided:

Subtilase JP170 (SEQ ID NO:1)

Subtilase Y (SEQ ID NO:2)

Subtilase SD-521 (SEQ ID NO:3)

Subtilase BPN' (SEQ ID NO:4)

20 Partiel sequence (SEQ ID NO:5)

Partiel sequence (SEQ ID NO:6)

Subtilase TY145 (SEQ ID NO:7)

#### BRIEF DESCRIPTION OF THE INVENTION

Now the inventors of the present invention disclose the three-dimensional structure of the subtilase JP170. This subtilase has large structural differences to the structures of the subtilisins BPN' and TY145.

Based on these differences the inventors have modified the amino acid sequence of subtilases having a JP170 type structure and subtilases having a BPN' type structure to obtain variants with improved properties. The variants have altered properties, such as increased activity at low temperatures, increased thermostability, increased specific activity at a given pH, altered Ca<sup>2+</sup> dependency, increased stability in the presence of other detergent ingredients (e.g. bleach, surfactants etc.) etc.

Accordingly, the object of the present invention is to provide a method for constructing subtilases having altered properties, in particular to provide a method for constructing subtilases having altered properties as described above.

Thus the present invention relates to a method for constructing a variant of a parent subtilase, wherein the variant has at least one altered property as compared to said parent subtilase, which method comprises:

- a) analyzing the three-dimensional structure of the subtilase to identify, on the basis of an evaluation of structural considerations in relation to a JP170 three dimensional structure, at least one amino acid residue or at least one structural region of the subtilase, which is of relevance for altering said property;
- b) modifying the DNA of the polynucleotide encoding the parent to construct a polynucleotide encoding a variant subtilase, which in comparison to the parent subtilase, has been modified by deletion, substitution or insertion of the amino acid residue or structural part identified in i) so as to alter said property;
- c) expressing the variant subtilase in a suitable host, and

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d) testing the resulting subtilase variant for said property.

More specifically the invention relates to a method of producing a subtilase variant, wherein the variant has at least one altered property as compared to a parent subtilase, which method comprises:

- a) producing a model structure of the parent subtilase on the three-dimensional structure of BPN', TY145 or JP170; or producing an actually determined threedimensional structure of the parent subtilase,
- b) comparing the model or actual three-dimensional structure of the parent subtilase to the JP170 structure by superimposing the structures through matching the CA, CB, C, O, and N atoms of the active site residues,
- c) identifying on the basis of the comparison in step b) at least one structural part of the parent subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
- d) modifying the nucleic acid sequence encoding the parent subtilase to produce a nucleic acid sequence encoding at least one deletion or substitution of one or more amino acids at a position corresponding to said structural part, or at least one inser-

tion of one or more amino acid residues in positions corresponding to said structural part;

- e) performing steps c) and d) iteratively N times, where N is an integer with the value of one or more;
- f) preparing the variant resulting from steps a) e);
- g) testing the properties of said variant; and
- h) optionally repeating steps a) g) recursively; and
- selecting a subtilase variant having at least one altered property as compared to the parent subtilase.
- j) expressing the modified nucleic acid sequence in a host cell to produce the variant subtilase;
- k) isolating the produced subtilase variant;
- I) purifying the isolated subtilase variant and
- m) recovering the purified subtilase variant.

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Although it has been described in the following that modification of the parent subtilase in certain regions and/or positions is expected to confer a particular effect to the thus produced subtilase variant, it should be noted that modification of the parent subtilase in any of such regions may also give rise to any other of the above-mentioned effects. For example, any of the regions and/or positions mentioned as being of particular interest with respect to, e.g., improved thermostability, may also give rise to, e.g., higher activity at a lower pH, an altered pH optimum, or increased specific activity, such as increased peptidase activity.

Further aspects of the present invention relates to variants of a subtilase, the DNA encoding such variants and methods of preparing the variants. Still further aspects of the present invention relates to the use of the variants for various industrial purposes, in particular as an additive in detergent compositions. Other aspects of the present invention will be apparent from the below description as well as from the appended claims.

#### DEFINITIONS

Prior to discussing this invention in further detail, the following terms and conventions will first be defined.

For a detailed description of the nomenclature of amino acids and nucleic acids, we refer to WO 00/71691 page 5, hereby incorporated by reference. A description of the nomenclature of modifications introduced in a polypeptide by genetic manipulation can be found in WO 00/71691 page 7-12, hereby incorporated by reference.

The term "subtilases" refer to a sub-group of serine protease according to Siezen *et al.*, *Protein Engng.* 4 (1991) 719-737 and Siezen et al. *Protein Science* 6 (1997) 501-523. Serine proteases or serine peptidases is a subgroup of proteases characterised by having a serine in the active site, which forms a covalent adduct with the substrate. Further the subtilases (and the serine proteases) are characterised by having two active site amino acid residues apart from the serine, namely a histidine and an aspartic acid residue.

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Subtilases are defined by homology analysis of more than 170 amino acid sequences of serine proteases previously referred to as subtilisin-like proteases. The subtilases may be divided into 6 sub-divisions, i.e. the Subtilisin family, the Thermitase family, the Proteinase K family, the Lantibiotic peptidase family, the Kexin family and the Pyrolysin family.

The Subtilisin family (EC 3.4.21.62) may be further divided into 3 sub-groups, i.e. I-S1 ("true" subtilisins), I-S2 (highly alkaline proteases) and intracellular subtilisins. Definitions or grouping of enzymes may vary or change, however, in the context of the present invention the above division of subtilases into sub-division or sub-groups shall be understood as those described by Siezen et al., *Protein Engng.* 4 (1991) 719-737 and Siezen et al. *Protein Science* 6 (1997) 501-523.

The term "parent" is in the context of the present invention to be understood as a protein, which is modified to create a protein variant. The parent protein may be a naturally occurring (wild-type) polypeptide or it may be a variant thereof prepared by any suitable means. For instance, the parent protein may be a variant of a naturally occurring protein which has been modified by substitution, chemical modification, deletion or truncation of one or more amino acid residues, or by addition or insertion of one or more amino acid residues to the amino acid sequence, of a naturally-occurring polypeptide. Thus the term "parent subtilase" refers to a subtilase which is modified to create a subtilase variant.

The term "variant" is in the context of the present invention to be understood as a protein which has been modified as compared to a parent protein at one or more amino acid residues.

The term "modification(s)" or "modified" is in the context of the present invention to

be understood as to include chemical modification of a protein as well as genetic manipulation of the DNA encoding a protein. The modification(s) may be replacement(s) of the amino acid side chain(s), substitution(s), deletion(s) and/or insertions in or at the amino acid(s) of interest. Thus the term "modified protein", e.g. "modified subtilase", is to be understood as a protein which contains modification(s) compared to a parent protein, e.g. subtilase.

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"Homology" or "homologous to" is in the context of the present invention to be understood in its conventional meaning and the "homology" between two amino acid sequences should be determined by use of the "Similarity" defined by the GAP program from the University of Wisconsin Genetics Computer Group (UWGCG) package using default settings for alignment parameters, comparison matrix, gap and gap extension penalties. Default values for GAP penalties, i.e. GAP creation penalty of 3.0 and GAP extension penalty of 0.1 (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711). The method is also described in S.B. Needleman and C.D. Wunsch, Journal of Molecular Biology, 48, 443-445 (1970). Identities can be extracted from the same calculation. The homology between two amino acid sequences can also be determined by "identity" or "similarity" using the GAP routine of the UWGCG package version 9.1 with default setting for alignment parameters, comparison matrix, gap and gap extension penalties can also be applied using the following parameters: gap creation penalty = 8 and gap extension penalty = 8 and all other parameters kept at their default values. The output from the routine is besides the amino acid alignment the calculation of the "Percent Identity" and the "Similarity" between the two sequences. The numbers calculated using UWGCG package version 9.1 is slightly different from the version 8.

The term "position" is in the context of the present invention to be understood as the number of an amino acid in a peptide or polypeptide when counting from the N-terminal end of said peptide/polypeptide. The position numbers used in the present invention refer to different subtilases depending on which subgroup the subtilase belongs to.

As mentioned above the alkaline subtilases KP43, KP1790, KP9860, Y, SD-521 and E1 belong to the JP170 subgroup, based on sequence homology. Due to the extensive homology only subtilase Ya and SD-521 are in Fig. 1 aligned with JP170. The JP170 subtilase, Y subtilase and SD-521 subtilase are numbered according to SEQ ID NO:1, SEQ ID NO:2 and SEQ ID NO:3, respectively.

The invention, however, is not limited to variants of these particular subtilases but extends to parent subtilases, especially of the JP170 type, containing amino acid residues at positions which are "equivalent" to the particular identified residues in the JP170 subtilase.

A residue (amino acid) position of a JP170 type subtilase is equivalent to a residue (position) of the JP170 subtilase, if it is either homologous (i.e., corresponding in position in either primary or tertiary structure) or analogous to a specific residue or portion of that residue in the JP170 subtilase (i.e., having the same or similar functional capacity to combine, react, or interact chemically).

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In order to establish homology to primary structure, the amino acid sequence of a precursor protease is directly compared to the JP170 subtilase primary sequence by aligning the amino acid sequence of an isolated or parent wild type enzyme with a suitable well-known (standard) enzyme of the same group or class of enzymes to define a frame of reference. This type of numbering has been used in numerous patent applications relating to subtilisins of the I-S1 and I-S2 subgroups with subtilisin BPN' as the standard subtilisin.

If nothing else is indicated herein, in the present instance the JP170 subtilase has been chosen as standard.

In order to establish homology to the tertiary structure (3D structure) of JP170, the 3D structure based alignment in Fig. 1 has been provided. By using this alignment the amino acid sequence of a precursor JP170 type subtilase may be directly correlated to the JP170 primary sequence. For a novel JP170 type subtilase, the (3D based) position corresponding to a position in JP170 is found by

- i) identifying the JP170 type subtilase from the alignment of Fig. 1 that is most homologous to the novel sequence,
- ii) aligning the novel sequence with the sequence identified to find the corresponding position in the JP170 type subtilase from Fig. 1, and
- iii) establishing from Fig. 1 the corresponding position in JP170.

For comparison and finding the most homologous sequence the GAP program from GCG package as described below are used.

The alignment can as indicated above be obtained by the GAP routine of the GCG package version 8 to number the variants using the following parameters: gap creation penalty = 3 and gap extension penalty = 0.1 and all other parameters kept at their default values.

The alignment may define a number of deletions and insertions in relation to the sequence of JP170. In the alignment deletions are indicated by asterixes (\*) in the referenced sequence, and the referenced enzyme will be considered to have a gap at the position in question. Insertions are indicated by asterixes (\*) in the JP170 sequence, and the positions in the referenced enzyme are given as the position number of the last amino acid residue where a corresponding amino acid residue exists in the standard enzyme with a lower case letter appended in alphabetical order, e.g. 82a, 82b, 82c, 82d.

In case the referenced enzyme contains a N- or C-terminal extension in comparison to JP170; an N-terminal extension is given the position number 0a, 0b, etc. in the direction of the N-terminal; and a C-terminal extension will be given either the position number of the C-terminal amino acid residue of JP170 with a lower case letter appended in alphabetical order, or simply a continued consecutive numbering.

Thus for comparisons JP170 type subtilases are numbered by reference to the positions of the JP170 subtilase (SEQ ID NO: 1) as provided in Fig. 1. The position is then indicated as "corresponding to JP170".

Subtilases belonging to the BPN' subgroup refers to the positions of Subtilisin Novo (BPN') from *B. amyloliquefaciens* (SEQ ID NO:4).

Subtilases belonging to the TY145 subgroup refers to the positions of the TY145 subtilase (SEQ ID NO:7), see also PCT/DK2004/000066.

#### DETAILED DESCRIPTION OF THE INVENTION

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Despite the great homology of the subtilases described above the inventors of the present invention have elucidated the three-dimensional structure of JP170, SEQ ID NO:1 by X-ray crystallography and found that there are several differences between this and the three-dimensional structure of BPN'. The inventors of the present invention have further compared the sequence homology of subtilases belonging to the Subtilisin subgroup. This is shown in Figure 3 of the present invention.

On the basis of this comparison the inventors of the present invention suggest to divide the Subtilisin subgroup so that the JP170 type subtilases become a separate subgroup in addition to the subgroups of BPN' subtilases and TY145 subtilases PCT/DK2004/000066.

## JP170 type subtilases

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The term "JP170 subtilase" or "JP170 type subtilase" should in the context of the present invention be understood as a subtilase belonging to the Subtilisin group according to Siezen et al. *Protein Science* 6 (1997) 501-523 and which has at least 58% homology to JP170, SEQ ID NO:1. In particular a JP170 type subtilase may have at least 60% homology to SEQ ID NO:1, such as at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to JP170, i.e. to SEQ ID NO:1. Thus, among others the alkaline proteases KP43, KP1790, KP9860, Protease Ya, Protease E-1 and SD-521 are subtilases belonging to the JP170 subgroup of subtilases.

A JP170 subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of JP170, i.e. it may be homologous to the three-dimensional structure defined by the structure coordinates in Appendix 1.

As it is well-known to a person skilled in the art that a set of structure coordinates for a protein or a portion thereof is a relative set of points that define a shape in three dimensions, it is possible that an entirely different set of coordinates could define an identical or a similar shape. Moreover, slight variations in the individual coordinates may have little or no effect on the overall shape.

These variations in coordinates may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates of JP170 (Appendix 1) may be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above. Alternatively, said variations may be due to differences in the primary amino acid sequence.

If such variations are within an acceptable standard error, such as 0.8 Å, as compared to the structure coordinates of Appendix 1, said three-dimensional structure is within the context of the present invention to be understood as being homologous to the structure of Appendix 1. The standard error may typically be measured as the root mean square deviation of e.g. conserved backbone residues, where the term "root mean square deviation" (RMS) means the square root of the arithmetic mean of the squares of the deviations from

the mean.

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As it is also well-known to a person skilled in the art that within a group of proteins which have a homologous structure there may be variations in the three-dimensional structure in certain areas, sub-structures or domains of the structure, e.g. loops, which are not or at least only of a small importance to the functional domains of the structure, but which may result in a big root mean square deviation of the conserved residue backbone atoms between said structures.

Thus it is well known that a set of structure coordinates is unique to the crystallised protein. No other three dimensional structure will have the exact same set of coordinates, be it a homologous structure or even the same protein crystallised in a different manner. There are natural fluctuations in the coordinates. The overall structure and the inter-atomic relationship can be found to be similar. The similarity can be discussed in terms of root mean square deviation of each atom of a structure from each "homologous" atom of another structure. However, only identical proteins have the exact same number of atoms. Therefore, proteins having a similarity below 100% will normally have a different number of atoms, and thus the root mean square deviation can not be calculated on all atoms, but only the ones that are considered "homologous". A precise description of the similarity based on the coordinates is thus difficult to describe and difficult to compute for homologous proteins. Regarding the present invention, similarities in 3D structure of different subtilases can be described by the content of homologous structural elements, and/or the similarity in amino acid or DNA sequence. For sequences having no deletions or insertions a RMS for the CA carbon atoms can be calculated.

Optionally a JP170 type subtilase is further characterised as comprising the following structural characteristics:

- a) a twisted beta-sheet with 7 strands.
- b) six alpha helices,
- c) at least three ion-binding sites, and not comprising the Strong and Weak ion-binding site of the BPN' like subtilases

Further the isolated nucleic acid sequence encoding a JP170 subtilase of the invention hybridizes with a complementary strand of a nucleic acid sequence encoding the amino acid sequence of SEQ ID NO:1 preferably under low stringency conditions, at least under medium stringency conditions, at least under medium/high stringency conditions, at least under very high stringency conditions.

Suitable experimental conditions for determining hybridization at low, medium, or high stringency conditions between a nucleotide probe and a homologous DNA or RNA sequence involves presoaking of the filter containing the DNA fragments or RNA to hybridize in 5 x SSC (Sodium chloride/Sodium citrate, Sambrook et al. 1989) for 10 min, and prehybridization of the filter in a solution of 5 x SSC, 5 x Denhardt's solution (Sambrook et al. 1989), 0.5 % SDS and 100 µg/ml of denatured sonicated salmon sperm DNA (Sambrook et al. 1989), followed by hybridization in the same solution containing a concentration of 10ng/ml of a random-primed (Feinberg, A. P. and Vogelstein, B. (1983) *Anal. Biochem.* 132:6-13), <sup>32</sup>P-dCTP-labeled (specific activity > 1 x 10<sup>9</sup> cpm/µg) probe for 12 hours at ca. 45°C. The filter is then washed twice for 30 minutes in 2 x SSC, 0.5 % SDS at least \* 55°C (low stringency), more preferably at least 60°C (medium stringency), still more preferably at least 65°C (medium/high stringency), even more preferably at least 70°C (high stringency), and even more preferably at least 75°C (very high stringency).

# BPN' subtilases

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A BPN' subtilase or BPN' type subtilase is in the context of the present invention to be understood as a subtilase belonging to the Subtilisin group according Siezen et al. Siezen et al. *Protein Science* 6 (1997) 501-523 and which has at least 61% homology to SEQ ID NO:4. In particular a BPN' subtilase may have at least 65%, such as at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to BPN', i.e. to SEQ ID NO:4.

Further the isolated nucleic acid sequence encoding a BPN' subtilase of the invention hybridizes with a complementary strand of the nucleic acid sequence encoding the amino acid sequence of SEQ ID NO:4 preferably under low stringency conditions, at least under medium stringency conditions, at least under medium/high stringency conditions, at least under very high stringency conditions.

In one embodiment of the present invention a BPN' subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of BPN' as defined by the structure coordinates given in PDB Nos. 1SBT and 1GNS (Protein Data Bank), or one of the several other structures of BPN' that are accessible from the Protein Data Bank. Variations between homologous structures may occur for several reasons as described above. Thus a BPN' subtilase within the context of the present invention is to

be understood as any subtilase having the structural characteristics pertaining to the BPN' subtilases as described above, and in addition such subtilases do preferably not have further structural characteristics which are not present in the BPN' subtilases as described herein. In the context of the present invention a BPN' type subtilase has two ion-binding sites. A BPN' like subtilase may, in the context of the present invention, belong to branch I-S of the subtilisins i.e. to branch I-S1, the "true" subtilisins or I-S2, the highly alkaline proteases (Siezen et al., *Protein Engng.* 4 (1991) 719-737).

Examples of BPN' type subtilases include the subtilisin 309 (PDB NO:1SVN, SAVI-NASE®, NOVOZYMES A/S) and subtilisin Carlsberg (ALCALASE®, NOVOZYMES A/S), among others.

In connection with Figure 1 of R.J. Siezen and J.A.M Leunissen (Protein science, Vol. 6 (3), pp. 501-523, 1997) page 502 a structure of subtilases is described as: A subtilase consists of 6-8 helices, 11 strands of which 7 are central in a twisted beta-sheet. Two ion-binding sites are mentioned, the so called "Strong" and "Weak" calcium-binding sites. It was later discovered that for some structures (subtilisin DY PDB no. 1BH6, 1998), the Weak calcium-binding site was shown to be a Na (sodium) binding site when the calcium concentration in the crystallization medium was low. Thus, in the following we refer to ion-binding sites instead of calcium-binding sites.

#### 20 TY145 subtilases

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A TY145 subtilase or TY145 type subtilase is in the context of the present invention to be understood as a subtilase which has at least 63% homology to SEQ ID NO:7. In particular said TY145 subtilase may have at least 65%, such as at least 70%, at least 74%, at least 80%, at least 83%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to TY145, i.e. to SEQ ID NO:7.

In one embodiment of the present invention a TY145 subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of TY145 as defined by the structure coordinates given in PCT/DK2004/000066. Variations between homologous structures may occur for several reasons as described above. Thus a TY145 subtilase within the context of the present invention is to be understood as any subtilase having the structural characteristics pertaining to the TY145 subtilases as described above, and in addition such subtilases do preferably not have further structural characteristics.

tics which are not present in the TY145 subtilases as described herein.

Typically a TY145 subtilase further comprises the following structural characteristics:

- a) a twisted beta-sheet with 7 strands,
- b) six alpha helices,

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c) at least three ion-binding sites, wherein the Strong ion-binding site of the BPN' type subtiliases is not present,

Examples of subtilases of the TY145 type include the TY145 subtilase, the psychrophilic subtilisin protease S41 derived from the Antarctic Bacillus TA41, herein also called TA41 subtilase (Davail S et al., 1994, J. Biol. Chem., 269, 17448-17453), and the psychrophilic subtilisin protease S39 derived from the Antarctic Bacillus TA39, herein also called TA39 subtilase (Narinx E et al., 1997, Protein Engineering, 10 (11), 1271-1279).

# Three-dimensional structure of JP170 subtilases

The JP170 subtilase was used to elucidate the three-dimensional structure forming the basis for the present invention.

The structure of JP170 was solved in accordance with the principle for x-ray crystal-lographic methods, for example, as given in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989.

The structural coordinates for the solved crystal structure of JP170 are given in standard PDB format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT) as set forth in Appendix 1. It is to be understood that Appendix 1 forms part of the present application. In the context of Appendix 1, the following abbreviations are used: CA refers to c-alpha (carbon atoms) or to calcium ions, (however to avoid misunderstandings we normally use the full names "c-alpha atoms" and "calcium" or "ion" in the present specification). Amino acid residues are given in their standard three-letter code. The attached structural coordinates contain the protease structure, and an inhibitor structure CI2 as well as water molecules. The protease coordinates has a chain identification called A, whereas the CI2 inhibitor is called B, the calcium ions are called C, and the water is W. In the following the positions of the mentioned residues refer to the sequence of JP170 as disclosed in SEQ ID NO:1.

The JP170 structure consists of two domains, a catalytic domain and a C-terminal domain.

The structure of the catalytic domain shows the same overall fold as found in the S8

family of subtilisins. The structure comprises a twisted beta-sheet with 7 strands arranged in the following sequential order S2, S3, S1, S4, S5, S6, S7.

There are six alpha helices in the catalytic domain structure of which number H1 contains residues 9-17, H2 contains residues 68-76, H3 contains residues 110-119, H4 contains residues 139-150, H5 contains residues 253-273 and H6 contains residues 281-291.

The C-terminal domain comprises a strand motif, a so called "beta sandwich" consisting of sheets a and b. The sheet in this domain is combined of strands in an anti-parallel fashion, whereas the strand in the catalytic domain is combined in parallel. The sequential order of the strands can be denoted as: S1a-S1b-S3a-S3b-S4b-S4a-S2b-S2a with the beta sandwich organised as to the two sheets S1a, S3a, S4a, S2a and S1b, S3b, S4b, S2b.

The JP170 subtilases were found to lack the well-known Strong and Weak ion-binding sites of the BPN' subtilases. However, the JP170 subtilases have three ion-binding sites which are not present in the BPN' subtilisin structures. This can be seen in the structural alignment presented in Fig. 2. These three ion-binding sites are hereinafter referred to as Site 1, which is placed in the catalytic domain, and Site 2 and 3 which are placed in the non-catalytic C-terminal domain.

Thus in relation to the atomic coordinates disclosed in Appendix 1, the ion-binding sites of JP170 are located at:

- Site 1 calcium atom named A601 CA
- Site 2 calcium atom named A603 CA, and
- Site 3 calcium atom named A602 CA in the PDB table (Appendix 1).

The position of an ion-binding site can be defined by the distance to four specific atoms in the core structure. The distance from the ion-binding site to the c-alpha atoms of the three active site residues has been chosen. Throughout the subtilases the residues Ser, His and Asp in the active site are highly conserved. In JP170 they are Asp30, His68 and Ser254. The fourth distance chosen is the distance to the c-alpha atom of the amino acid residue coming first after the active site serine residue in the sequence (herein after called "next to Ser"); in the 3D structure of JP170 it is Met255.

In a preferred embodiment of the present invention, the distance between:

30 a) ion-binding site 1 and

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- i) Asp c-alpha atom is 26.70-28.70Å,
- ii) His c-alpha atom is 22.10-24.10Å,
- iii) Ser c-alpha atom is 16.95-18.95Å,

- iv) next to Ser c-alpha atom is 15.30-17.30Å,
- b) ion-binding site 2 and
  - i) Asp c-alpha atom is 33.50-35.50Å,
  - ii) His c-alpha atom is 37-39Å,
  - iii) Ser c-alpha atom is 29.40-31.40Å,
  - iv) next to Ser c-alpha atom is 30.70-32.70Å,
- c) ion-binding site 3 and

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- i) Asp c-alpha atom is 41.50-43.50Å,
- ii) His c-alpha atom is 42.90-44.90Å,
- iii) Ser c-alpha atom is 34.50-36.50Å,
- iv) next to Ser c-alpha atom is 35-37Å.

Below the specific distances between the four chosen c-alpha atoms and the three ion binding sites of the JP170 subtilase; and the distances between the ion binding sites are given in Å:

	site 1	site 2	site 3
-Asp30	27.69	34.49	. 42.48
His68	23.12	38.03	43.87
Ser254	17.95	30.41	35.51
Met255	16.34	31.68	36.02
site 1	0	35.29	32.92
site 2	35.29	0	14.08
site 3	32.92	14.08	. 0

However, these distances may vary from one subtilase to the other. The present distances are given with a calcium ion in the structure. If a sodium ion was bound instead the distances would be shifted a little bit. Generally the distances can vary  $\pm 0.80$ Å, preferably  $\pm 0.70$ Å,  $\pm 0.60$ Å,  $\pm 0.50$ Å,  $\pm 0.40$ Å, or most preferably  $\pm 0.30$ Å.

Further, in the JP170 like subtilases, the peptide structure circumscribing ion-binding site 1 up to a distance of 10 Å from the metal ion is composed of the amino acid residues placed in positions 183-189, 191-204 and 224-225.

The peptide structure circumscribing ion-binding site 2 up to a distance of 10 Å from the metal ion is composed of residues 378-393.

The peptide structure circumscribing ion-binding site 3 up to a distance of 10 Å from the metal ion is composed of residues 348, 350, 352, 363-370, 380-383, 391-400 and 414-420.

# 5 Comparison to the I-S1 and I-S2 subgroups (BPN' like subtilases)

In comparison to the BPN' like subtilase structures the structure of the JP170 like subtilases can be divided into a "core subtilase-like" region, an "intermediate" region and a "nonhomologous" region.

The active site can be found in the core subtilase-like region, which is structurally closely related to the BPN' structures. The core subtilase-like region is composed of residues 17-34, 197-209 and 216-232, and contains the alpha-helix H3 and the central alphahelix H5 in which the active site serine residue is situated in the N-terminal part. The core subtilase-like region has an RMS lower than 1.2.

Outside the core subtilase-like region the structure of the JP170 like subtilase differs from the BPN' structures to a greater extent.

The intermediate region consists of residues 42-46, 150-186, 245-272 and 278-296. The intermediate region has an RMS bigger than 1.2 and less than 1.8. The relationships between the three-dimensional structure and functionality are potentially difficult to predict in this region of the JP170 like subtilases.

The nonhomologous region consists of residues 1-16, 35-41, 47-149, 187-196, 210-215, 233-244, 273-277 and 297-316. The nonhomologous region has a RMS higher than 1.8. The relationships between the three-dimensional structure and functionality are very difficult to predict in this region of the JP170 like subtilases.

Many loops in the 3D structure of the JP170 like subtilases differ significantly from the BPN' type structures, both in length and in content of amino acid residues. The following loops or protein sequence stretches of JP170 are compared to Savinase (BPN' numbering in parenthesis, (cf. Fig. 4)):

G32-H43 (G34-H39)

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E44-Y54 (P40-A48)

G57-G67 (V51-G63)

N79-N82 (I75-V81)

196-P107 (V95-S105)

A108-S119 (106-N117)

A131-Y137 (S128-S132)

T138-D152 (A133-G146)

E162-I169 (S156-I165)

G173-T180 (A169-A176)

E185-N199 (D181-N184)

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G208-D218 (G193-D197)

S232-K246 (G211-T213)

D294-N303 (S256-L262)

The loops N79-N82 (I75-V81) and G208-D218 (G193-D197) are in contact with a ion-binding site in Savinase, but not in JP170. Similarly the loop E185-N199 (D181-N184) is in contact with a ion-binding site in JP170, but not in Savinase. This knowledge opens for possibilities of adding or removing ion-binding sites to subtilases of the JP170 and BPN' like types.

A good example of the difference is the loop S232-K246 in JP170 which has 15 residues compared to the corresponding BPN' type loop G211-T213 (in Savinase), which has only three residues. In the JP170 like subtilases, the loop folds back to the substrate binding site, especially the P' parts of the substrate binding site. The loop is situated close to the substrate as illustrated by the CI2 inhibitor bound in the 3D structure attached (Appendix 1).

The location of loop S232-K246 in JP170 can be described in relation to the four specific residues as described above. The distance from the CA atom of residue W240 in the loop to the CA atoms of the active site residues are:

Residue H68 D30 S254 M255 Distance, Å 11.45 18.51 13.06 11.94

As mentioned above, distances like these can vary  $\pm 0.80$ Å, preferably  $\pm 0.70$ Å,  $\pm 0.60$ Å,  $\pm 0.50$ Å,  $\pm 0.40$ Å, or most preferably  $\pm 0.30$ Å.

Furthermore, distances from the residues of JP170 loop S232-K246 to atoms of the CI2 inhibitor can be calculated. These distances are:

from CA atom of W240 to CA atom of R62 in CI2 is 7.49Å,

from CA atom of F239 to CA atom of R62 in Cl2 is 8.39Å,

from CA atom of S238 to CA atom of R62 in Cl2 is 8.42Å,

from CA atom of S237 to CA atom of R62 in Cl2 is 9.44Å,

from CA atom of S238 to CA atom of E60 in Cl2 is 9.42Å.

The distances from JP170 active site residue S254 to atoms of the Cl2 inhibitor, as placed in the 3D coordinates of Appendix 1, are:

from CA atom of S254 to CA atom of E60 in Cl2 is 5.25Å, from CA atom of S254 to CA atom of R62 in Cl2 is 11.55Å, from CA atom of S254 to CA atom of T58 in Cl2 is 7.06Å, from CA atom of S254 to CA atom of M59 in Cl2 is 4.71Å.

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The distances can vary  $\pm 0.80$ Å, preferably  $\pm 0.70$ Å,  $\pm 0.60$ Å,  $\pm 0.50$ Å,  $\pm 0.40$ Å, or most preferably  $\pm 0.30$ Å.

A preferred JP170 like subtilase variant has a deletion in the region S232-K246, and the subsequent insertion of one or more residues to partly or completely remove the loop. Preferred variants comprises the deletion of L233-S245 + insertion of Asn, deletion of L233-D244 + insertion of Gly or deletion of S232-D244 + insertion of Gly.

Similar considerations can be made in respect of differences to the TY145 structure.

# Homology building of JP170, BPN' and TY145 subtilases

A model structure of a JP170 type subtilase, a BPN' type subtilase or a TY145 type subtilase can be built using the Homology program or a comparable program, e.g., Modeller (both from Molecular Simulations, Inc., San Diego, CA). The principle is to align the amino acid sequence of a protein for which the 3D structure is known with the amino acid sequence of a protein for which a model 3D structure has to be constructed. The structurally conserved regions can then be built on the basis of consensus sequences. In areas lacking homology, loop structures can be inserted, or sequences can be deleted with subsequent bonding of the necessary residues using, e.g., the program Homology. Subsequent relaxing and optimization of the structure should be done using either Homology or another molecular simulation program, e.g., CHARMm from Molecular Simulations.

# Methods for designing JP170, BPN', and TY145 subtilase variants

Comparisons of the molecular dynamics of different proteins can give a hint as to which domains are important or connected to certain properties pertained by each protein.

Thus the present invention relates to a method for constructing a variant of a parent

subtilase, wherein the variant has at least one altered property as compared to said parent subtilase, which method comprises:

- a) analyzing the three-dimensional structure of the parent subtilase to identify, on the basis of an evaluation of structural considerations in relation to a JP170 three dimensional structure, at least one amino acid residue or at least one structural region of the subtilase, which is of relevance for altering said property;
- b) modifying the DNA of the polynucleotide encoding the parent to construct a polynucleotide encoding a variant subtilase, which in comparison to the parent subtilase, has been modified by deletion, substitution or insertion of the amino acid residue or structural part identified in i) so as to alter said property;
- c) expressing the variant subtilase in a suitable host, and

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d) testing the resulting subtilase variant for said property.

More specifically the invention relates to a method of producing a subtilase variant, wherein the variant has at least one altered property as compared to a parent subtilase, which method comprises:

- a) producing a model structure of the parent subtilase on the three-dimensional structure of BPN', TY145 or JP170; or producing an actually determined threedimensional structure of the parent subtilase,
- b) comparing the model or actual three-dimensional structure of the parent subtilase to the JP170 structure by superimposing the structures through matching the CA, CB,
   C, O, and N atoms of the active site residues,
- c) identifying on the basis of the comparison in step b) at least one structural part of the parent subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
- d) modifying the nucleic acid sequence encoding the parent subtilase to produce a nucleic acid sequence encoding at least one deletion or substitution of one or more amino acids at a position corresponding to said structural part, or at least one insertion of one or more amino acid residues in positions corresponding to said structural part;
- e) performing steps c) and d) iteratively N times, where N is an integer with the value of one or more;
- f) preparing the variant resulting from steps a) e);

- g) testing the properties of said variant; and
- h) optionally repeating steps a) g) recursively; and
- i) selecting a subtilase variant having at least one altered property as compared to the parent subtilase.
- j) expressing the modified nucleic acid sequence in a host cell to produce the variant subtilase;
- k) isolating the produced subtilase variant;

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- I) purifying the isolated subtilase variant and
- m) recovering the purified subtilase variant.

The present invention thus generally relates to the use of the JP170 structure as provided herein for the identification of desired modifications in subtilases of any of the three subtilisin types, the BPN' types (I-S1 and I-S2 subgroups), the TY145 types and the JP170 types through modelling the 3-D structure of a parent subtilase to the type it belongs to and subsequent comparison thereof to the JP170 3-D structure, or in instances where the 3-D structure of the parent subtilase is actually known by comparison thereof to the JP170 3-D structure.

Based on this comparison at least one residue in the parent subtilase is selected for modification by substitution, deletion or insertion in order to provide a subtilase variant with altered properties in comparison to the parent subtilase.

In one embodiment the parent subtilase may therefore belong to the sub-group I-S1, preferably selected from the group consisting of ABSS168, BASBPN, BSSDY, and BLSCAR, or functional variants thereof having retained the characteristic of sub-group I-S1.

In another embodiment the parent subtilase belongs to the sub-group I-S2, preferably selected from the group consisting of BLS147, BLS309, BAPB92, and BYSYAB, or functional variants thereof having retained the characteristic of sub-group I-S2.

In a further embodiment the parent subtilase belongs to the TY145 type subgroup, preferably selected from the group comprising TY145, protease S41 also called TA41 protease S39 also called TA39 subtilase, etc.

Specifically the parent subtilase belongs to the JP170 type subgroup, preferably selected from the group comprising JP170, KP43, KP9860, Protease E-1, Protease Ya, Protease SD-521, etc.

A further embodiment of the invention relates to a method of producing a JP170 type subtilase variant, wherein the variant has at least one altered property as compared to a parent subtilase, which method comprises:

- a) producing a model structure of the parent JP170 type subtilase on the threedimensional structure of JP170; or producing an actually determined threedimensional structure of the parent subtilase,
- b) comparing the model or actual three-dimensional structure of the parent JP170 type subtilase to the BPN' or TY145 structure by superimposing the structures through matching the CA, CB, C, O, and N atoms of the active site residues,
- c) identifying on the basis of the comparison in step b) at least one structural part of the parent JP170 type subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
- d) modifying the nucleic acid sequence encoding the parent JP170 type subtilase to produce a nucleic acid sequence encoding at least one deletion or substitution of one or more amino acids at a position corresponding to said structural part, or at least one insertion of one or more amino acid residues in positions corresponding to said structural part;
- e) performing steps c) and d) iteratively N times, where N is an integer with the value of one or more;
- f) preparing the JP170 type subtilase variant resulting from steps a) e);
- g) testing the properties of said variant; and

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- h) optionally repeating steps a) g) recursively; and
- i) selecting a JP170 type subtilase variant having at least one altered property as compared to the parent subtilase.
- j) expressing the modified nucleic acid sequence in a host cell to produce the variant subtilase;
- k) isolating the produced JP170 type subtilase variant;
- I) purifying the isolated subtilase variant and
- m) recovering the purified subtilase variant.

The invention also comprises the protease variants produced by the above methods.

As described above the three-dimensional structure of JP170 subtilases as provided in Appendix 1 indicates the presence of three ion-binding sites not present in the BPN' subtilisin structures, thus lacking the Strong and Weak ion-binding site of the BPN' subtilases. Stability of ion-binding sites is important for the functionality of the enzyme. Therefore alterations of the ion-binding sites are likely to result in alterations of the stability of the enzyme.

# Improved stability

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Stabilisation of a JP170 subtilase may possibly be obtained by alterations in the positions close to the ion-binding sites. Thus in one embodiment of the method of the invention step (c) above identifies amino acid residue positions located at a distance of 10Å or less to the ion-binding site of the JP170 type parent, preferably positions located at a distance of 6 Å or less.

Thus a preferred variant of the present invention has a modification in one or more of the positions located at a distance of 10Å to the ion-binding sites of JP170 (SEQ ID NO:1). These positions are:

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Site 1: 183-189 (i.e. positions 183, 184, 185, 186, 187, 188, 189),
191-204 (i.e. positions 191, 192, 193, 194, 195, 196, 197, 198, 199,
20 200, 201, 202, 203, 204),
224-225;

Site 2: 378-393 (i.e. positions 378, 379, 380, 381, 382, 383, 384, 385, 386, 387,
388, 389, 390, 391, 392, 393);
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Site 3: 348, 350, 352, 363-370 (i.e. positions 363, 364, 365, 366, 367, 368, 369, 370), 380-383 (i.e. positions 380, 381, 382, 383), 391-400 (i.e. positions 391, 392, 393, 394, 395, 396, 397, 398, 399, 400), 414-420 (i.e. positions 414, 415, 416, 417, 418, 419, 420).

Corresponding positions in other JP170 type subtilases may be identified as disclosed above or by using Fig. 1 herein..

In detergent compositions calcium chelaters contribute to removal of calcium from the subtilases with subsequent inactivation of the enzyme as the result. To decrease the inactivation due to calcium removal of e.g. calcium chelaters variants with improved calcium stability was constructed.

Preferred variants stabilised in ion-binding site 1 are S193Q,Y; H200D,N and H200D,N+D196N.

Preferred variants stabilised in ion-binding site 2 are N390D and N391D, and preferred variants stabilised in ion-binding site 3 are G394N,Q,F,Y,S and W392S,N,Q.

#### Alteration of thermostability

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A variant with improved stability (typically increased thermostability) may be obtained by substitution with proline, introduction of a disulfide bond, altering a hydrogen bond contact, altering charge distribution, introduction of a salt bridge, filling in an internal structural cavity with one or more amino acids with bulkier side groups (in e.g. regions which are structurally mobile), substitution of histidine residues with other amino acids, removal of a deamidation site, or by helix capping.

# Regions with increased mobility:

The following regions of JP170 have an increased mobility in the crystal structure of the enzyme, and it is presently believed that these regions can be responsible for stability or activity of JP170. Especially thermostabilisation may possibly be obtained by altering the highly mobile regions. Improvements of the enzyme can be obtained by mutation in the below regions and positions. Introducing e.g. larger residues or residues having more atoms in the side chain could increase the stability, or, e.g., introduction of residues having fewer atoms in the side chain could be important for the mobility and thus the activity profile of the enzyme.

Two methods are used extract the highly mobile regions from a 3D structure. One is a molecular dynamics calculation of the isotropic fluctuations by using the program CHARMm from MSI (Molecular Simulations Inc.), and the other is an analysis of the B-factors. The B-factors are listed in Appendix 1 and give a value to the uncertainty of determination of the location of the various atoms of the structure. The uncertainty relates to the mobility of the atoms in the molecules in the crystal lattice. This mobility reflects the thermal motion of the atoms and thus indicates possible sites for thermostabilisation of the enzyme.

Thus, by analysing the B-factors taken from the coordinate file in Appendix 1, (see "X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989") the following mobile regions in the JP170 structure were determined:

```
(i.e. positions 13, 14, 15, 16, 17, 18),
      13-18
                    (i.e. positions 37, 38, 39, 40, 41, 42, 43),
      37-43
                    (i.e. positions 47, 48, 49, 50),
      47-50
      57-59
                    (i.e. positions 57, 58, 59),
      96-103
                    (i.e. positions 96, 97, 98, 99, 100, 101, 102, 103),
                    (i.e. positions 131, 132, 133, 134),
      131-134
      152-153
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                    (i.e. positions 162, 163, 164, 165, 166),
      162-166
                    (i.e. positions 188, 189, 190, 191, 192, 193, 194, 195),
      188-195
      210
                    (i.e. positions 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245,
      234-246
      246),
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                    (i.e. positions 372, 373, 374, 375, 376, 377, 378),
      372-378
                    (i.e. positions 387, 388, 389, 390, 391, 392),
      387-392
      406-407
      419.
             Molecular dynamics simulations at 300K and 400K of JP170 provided the following
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highly mobile regions:

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(i.e. positions 57, 58, 59, 60),
     57-60
     66-67,
                    (i.e. positions 98, 99, 100, 101, 102, 103),
     98-103
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     107-111
                    (i.e. positions 107, 108, 109, 110, 111),
     188-193
                    (i.e. positions 188, 189, 190, 191, 192, 193),
     236-240
                    (i.e. positions 236, 237, 238, 239, 240),
                    (i.e. positions 326, 327, 328, 329, 330, 331, 332),
     326-332
     337-342
                    (i.e. positions 337, 338, 339, 340, 341, 342),
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                    (i.e. positions 355, 356, 357, 358, 359, 360),
     355-360
                    (i.e. positions 372, 373, 374, 375, 376, 377),
     372-377
                    (i.e. positions 384, 385, 386, 387, 388).
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(i.e. positions 37, 38, 39, 40, 41, 42),

37-42

384-388

404-411 (i.e. positions 404, 405, 406, 407, 408, 409, 410, 411).

Thus, a preferred JP170 subtilase variant of the present invention has been modified in one or more of the above mentioned positions of SEQ ID NO:1. Further preferred variants comprises one or more alterations in the regions 57-60, 66-67, 107-111, 236-240, 326-332, 355-360, 372-377, 384-388, 404-411. Especially preferred is variant W240H,Y and variants modified in the region 355-360, such as variants comprising one or more of the modifications: G355A,S; S356T,N; T357N,Q,D,E,P; T358S; A359S,T,N,Q and S360T,N.

Variants modified in the region 355-360 may be produced in accordance with the method for random mutagenesis by use of the DOPE program as described herein. To obtain variants comprising 1-3 modifications in region 355-360 one may introduce the substitutions with the following frequencies:

	<u>wild-type</u>	<u>modified</u>	
	95%	5% G355A,S	
15	90%	10% S356T,N	
	80%	20% T357N,Q,D,E,P	
	90%	10% T358S	
	80%	20% A359S,T,N,Q	
	80%	20% S360T,N.	

# Disulfide bonds:

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A JP170 variant of the present invention with improved stability, e.g. thermostability, as compared to the parent JP170 subtilase may be obtained by introducing new interdomain or intra-domain bonds, such as by establishing inter- or intra-domain disulfide bridges.

Thus a further aspect of the present invention relates to a method for producing a variant of a parent JP170, wherein step (c) identifies amino acid residue positions in the parent JP170 type subtilase, the modification of which may create at least one disulfide bridge by insertion of or substitution with at least one Cys residue.

The below mentioned amino acid residues identified in the amino acid sequence of SEQ ID NO:1 are considered as being suitable for cysteine replacement. With one or more of these substitutions with cysteine, disulfide bridges may possibly form in a variant of JP170. The

substitutions are: G21C+A86C, V26C+A265C, G57C+G105C. G74C+A229C. A45C+G78C, Q111C+N143C, G160C+S170C, A286C+V349C, A27C+A122C, V72C+P258C. G78C+A229C, D98C+G104C, Q111C+Y147C, G135C+G167C, R142C+P354C, V144C+A178C, G182C+P217C, A183C+G223C, A195C+Y225C, F271C+P279C, A287C+A430C, A293C+T310C, E322C+S428C, S324C+A332C, S327C+P424C, D352C+N397C, G355C+T362C, G291C+S314C.

Preferred variants comprise one or more of the substitutions: G21C+A86C, V26C+A265C, G57C+G105C, G74C+A229C, Q111C+Y143C, G160C+S170C, A286C+V349C, A4C+P222C and A27C+A117C.

Similar residues suitable for cysteine replacement in subtilases homologous with JP170 can be elucidated by finding the homologous positions in the alignment of Figure 1. Concerning another JP170 like sequence the homologous positions suitable for cysteine replacement can be selected by aligning said JP170 like sequence with all of the sequences of Figure 1 using the GAP analysis method as described above. The suitable residues can then be selected in accordance with the homologous positions in the most homologous of SEQ ID's NO:1, 2 and 3 which are the sequences of the subtilases aligned in Figure 1.

#### Surface charge distribution

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A variant with improved stability (typically improved thermostability) as compared to the parent subtilase may be obtained by changing the surface charge distribution of the subtilase. For example, when the pH is lowered to about 5 or below histidine residues typically become positively charged and, consequently, unfavorable electrostatic interactions on the protein surface may occur. By engineering the surface charge of the subtilase one may avoid such unfavorable electrostatic interactions that in turn lead to a higher stability of the subtilase.

Charged amino acid residues are (a) positively charged: Lys, Arg, His (pH<5), Tyr (pH>9) and Cys (pH>10) and (b) negatively charged: Asp and Glu.

Therefore, a further aspect of the present invention relates to method for constructing a variant of a parent subtilase, the method comprising:

- a) identifying, on the surface of the parent subtilase, preferably a JP170 like or a BPN' like subtilase, at least one amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His;
- b) substituting, on the surface of the parent subtilase, at least one amino acid residue

selected from the group consisting of Asp, Glu, Arg, Lys and His with an uncharged amino acid residue;

- c) optionally repeating steps a) and b) recursively;
- d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b);
- e) preparing the variant resulting from steps a) d);
- f) testing the stability of said variant; and

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- g) optionally repeating steps a) f) recursively; and
- h) selecting a subtilase variant having increased stability as compared to the parent subtilase.

As will be understood by the skilled person it may also, in some cases, be advantageous to substitute an uncharged amino acid residue with an amino acid residue bearing a charge or, alternatively, it may in some cases be advantageous to substitute an amino acid residue bearing a charge with an amino acid residue bearing a charge of opposite sign. Thus, the above-mentioned method may easily be employed by the skilled person also for these purposes. In the case of substituting an uncharged amino acid residue with an amino acid residue bearing a charge the above-mentioned method may be employed the only difference being steps a) and b) which will then read:

- a) identifying, on the surface of the parent subtilase, at least one uncharged amino acid residue;
- b) substituting, on the surface of the parent subtilase, at least one uncharged amino acid residue with a charged amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His.

Also in the case of changing the sign of an amino acid residue present on the surface of the subtilase the above method may be employed. Again, compared to the above method, the only difference being steps a) and b) which, in this case, read:

- a) identifying, on the surface of the parent subtilase, at least one charged amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His;
- b) substituting, on the surface of the parent subtilase, at least one charged amino acid residue identified in step a) with an amino acid residue having an opposite charge.

Thus, Asp may be substituted with Arg, Lys or His; Glu may be substituted with Arg, Lys or His; Arg may be substituted with Asp or Glu; Lys may be substituted with Asp or Glu; and His may be substituted with Asp or Glu.

In order to determine the amino acid residues of a subtilase, which are present on the surface of the enzyme, the surface accessible area are measured using the DSSP program (Kabsch and Sander, *Biopolymers* (1983), 22, 2577-2637). All residues having a surface accessibilty higher than 0 0, 0.10, 0.20, 0.30, 0.35, 0.40, 0.45, 0.50, 0.55 or 0.60 are regarded a surface residue.

Among the amino acid residues found on the surface of JP170 using the above method are N79, N316, L381, K246, K9, K313 and K83. We consider the substitutions N79D, N316D and L381D of particular interest for stabilisation by introduction of salt bridges, whereas the substitutions K246R, K9R, K313R and K83R are of particular interest for the stabilisation at high pH.

Similar substitutions may be introduced in equivalent positions of other JP170 like subtilases.

# Substitution with proline residues

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Improved thermostability of a subtilase can be obtained by subjecting the subtilase in question to analysis for secondary structure, identifying residues in the subtilase having dihedral angles  $\phi$  (phi) and  $\psi$  (psi) confined to the intervals [-90°< $\phi$ <-40° and -180°< $\psi$ <180°], preferably the intervals [-90°< $\phi$ <-40° and 120°< $\psi$ <180°] or [-90°< $\phi$ <-40° and -50°< $\psi$ <10°] and excluding residues located in regions in which the subtilase is characterized by possessing  $\alpha$ -helical or  $\beta$ -sheet structure.

After the dihedral angles  $\phi$  (phi) and  $\psi$  (psi) for the amino acids have been calculated, based on the atomic structure in the crystalline subtilases, it is possible to select position(s) which has/have dihedral phi and psi angles favorable for substitution with a proline residue. The aliphatic side chain of proline residues is bonded covalently to the nitrogen atom of the peptide group. The resulting cyclic five-membered ring consequently imposes a rigid constraint on the rotation about the N-C $_{\alpha}$  bond of the peptide backbone and simultaneously prevents the formation of hydrogen bonding to the backbone N-atom. For these structural reasons, proline residues are generally not compatible with  $\alpha$ -helical and  $\beta$ -sheet secondary conformations.

If a proline residue is not already at the identified position(s), the naturally occurring

amino acid residue is substituted with a proline residue, preferably by site directed mutagenesis applied on a gene encoding the subtilase in question.

In the group of JP170 type subtilases proline residues can advantageously be introduced at positions 22, 44, 110, 139, 140, 166, 198, 201, 203, 231, 282, 356, 357 and 378. Accordingly, a preferred JP170 variant has one or more of the substitutions: Q22P, E44P, L110P, T139P, D140P, S166P I198P, V201P, Q203P, S231P, S282P, S356P, T357P and K378P. Especially preferred are variants comprising one or more of: E44P, Q203P and S356P.

## Improved activity of JP170 subtilases

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As mentioned, the JP170 subtilases differ greatly from the BPN' like subtilases in having a long apparently non-catalytic C-terminal. A possible truncation of JP170 is the removal of approx. 115 residues including two ion-binding sites, which can be obtained by deletion of or within the region 311-433, which is the non-catalytic C-terminal. Preferred deletions comprises the regions 317-433 or 315-433. Preferably the new C-terminal will be within the region of 311-325. Further, the deletion can be optimised with additional substitutions, such as one or more of L283N,Q; A290S,N and W306H,Y,K.

Preferred truncations comprise:

- a) deletion of region 317-433 and the substitutions L283N + A290S + W306H,
- b) deletion of region 315-433 and the substitutions L283N + A290S + W306H.

#### Substrate binding site

The substrate binding site is identified by the residues in contact with a substrate model, such as the CI2 inhibitor. The 3D structure coordinates of the JP170 subtilase with CI2 bound in the active site are provided in Appendix 1. Without being limited to any theory, it is presently believed that binding between a substrate and an enzyme is supported by favorable interactions found within a sphere 10 Å from the substrate molecule. Examples of such favorable bonds are hydrogen bonds, strong electrostatic interaction and/or hydrophobic interactions.

The following residues of the JP170 subtilase (SEQ ID NO:1), are within a distance of 10Å from the Cl2 inhibitor which is bound to the substrate binding site. These residues are thus believed to be involved in interactions with said substrate:

- 29-32, (i.e. residues 29, 30, 31, 32)
- 64-72, (i.e. residues 64, 65, 66, 67, 68, 69, 70, 71, 72)

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93,
                   (i.e. residues 96, 97, 98)
     96-98,
                   (i.e. residues 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110)
     100-110,
     113-114.
     127-136,
                   (i.e. residues 127, 128, 129, 130, 131, 132, 133, 134, 135, 136)
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                    (i.e. residues 138, 139, 140, 141)
     138-141,
     144, 157, 174,
     180-183,
                   (i.e. residues 180, 181, 182, 183)
     191, 193-194,
     202-207,
                   (i.e. residues 202, 203, 204, 205, 206, 207)
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     211,
                   (i.e. residues 223, 224, 225, 226)
     223-226,
     234-241,
                   (i.e. residues 234, 235, 236, 237, 238, 239, 240, 241)
                   (i.e. residues 249, 250, 251, 252, 253, 254, 255, 256, 257, 258).
     249-258
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In an embodiment of the present invention a variant comprises a modification in one or more of the above mentioned positions. A preferred variant is W129L.

#### JP170 with extra ion-binding site

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The Strong ion-binding site from the BPN' subtilases can be transplanted into JP170 (or other subtilases in JP170 subgroup) by deletion of N79-N82 and subsequent insertion of LNNSIGV (SEQ ID NO:5), followed by the substitutions E44P,T and/or R47Q.

# Removal of ion-binding site in JP170

By removing an ion-binding site it is possible to decrease the enzymes dependency of calcium in the media. The ion-binding sites in JP170 or other JP170 type subtilases can be removed with guidance from information about the three-dimensional structures of other related subtilases, such as a BPN' type subtilase, such as Savinase or BPN', and a TY145 type subtilase.

Removal of ion-binding site 1 can be done by deletion of N186-N199 and subsequent insertion of at least three amino acid residues – or stated differently by the substitution of a region comprising from 3 to 6 amino acid residues for the region comprising 14 amino acid residues in positions 186 to 199, preferably the sequence of the substituting re-

gion is SSN (SEQ ID NO:6). Preferably, but not mandatory one or both of the substitutions I7Q and V3Y is further added.

The ion-binding site 1 can be removed from a wild-type JP170 subtilase or a JP170 subtilase truncated as described above.

# Subtilases free of ion-binding sites

Similarly, information about the three-dimensional structures of JP170 type subtilases and TY145 type subtilases can be used to remove the Strong and Weak ion-binding sites in BPN' type subtilases, or the ion-binding sites in TY145 type subtilases may be removed on the basis of structural information about the JP170 and BPN' types of subtilases.

Using Savinase as an example, the removal can be done by altering the loops A194-L196 (weak ion-binding site) and L75-L82 (strong ion-binding site) either by a) insertion or deletion of a number of amino acid residues in the loops or b) by deletion of the entire loop or part of the loop and subsequent insertion of a number of residues from a corresponding loop of a JP170 or TY145 like subtilase.

Preferably the ion-binding sites of Savinase can be removed by either

- i) full or partial deletion of the region A194-L196 (BPN' numbers) and insertion of three or more residues chosen from JP170 positions P209-P217, and
- ii) full or partial deletion of the region L75-L82 (BPN' numbers) and insertion of at least one residue chosen from TY145 positions H83-Y92

or

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- i) full or partial deletion of the region A194-L196 (BPN' numbers) and insertion of three or more residues chosen from JP170 positions P209-P217 and
- ii) full or partial deletion of the region L75-L82 (BPN' numbers) and insertion of at least one residues chosen from JP170 positions N79-K83.

#### Removal of critical oxidation sites

In order to increase the stability of a JP170 type subtilase protease it may be advantageous to substitute or delete critical oxidation sites, such as methionines, with other amino acid residues which are not subject to oxidation.

Accordingly, in a further embodiment the present invention relates to an RP-II protease variant, in which one or more amino acid residues susceptible to oxidation, especially methionine residues exposed to the surface of the molecule, is/are deleted or replaced with another amino acid residue less susceptible to oxidation. The amino acid residue less susceptible to oxidation may for instance be selected from the group consisting of A, E, N, Q, I, L, S and K.

Specific such variants comprises at least one of the deletions or substitutions M42{\*,S,A,N,Q,K}; M85{\*,S,A,N,Q,K}; M97{\*,S,A,N,Q,K}; M153{\*,S,A,N,Q,K}; M220{\*,S,A,N,Q,K}; M250{\*,S,A,N,Q,K}; and M255{\*,S,A,N,Q,K} of the JP170 protease; the deletions or substitutions M42{\*,S,A,N,Q,K}; M85{\*,S,A,N,Q,K}; M97{\*,S,A,N,Q,K}; M153{\*,S,A,N,Q,K}; M250{\*,S,A,N,Q,K}; and M255{\*,S,A,N,Q,K} of the SD-521 and Ya proteases.

## Stabilization by modification of Asn-Gly pairs

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It is known that at alkaline pH, the side chain of Asn may interact with the NH group of a sequential neighbouring amino acid to form an isoAsp residue where the backbone goes through the Asp side chain. This will leave the backbone more vulnerable to proteolysis. The deamidation is much more likely to occur if the residue that follows is a Gly. Changing the Asn in front of the Gly or the Gly will prevent this from happening and thus improve the stability, especially as concerns thermo- and storage stability.

The invention consequently further relates to a subtilase, in which the modifications indicated above are either or both residues of any of the Asn-Gly sequence appearing in the amino acid sequence of the parent RP-II protease is/are deleted or substituted with a residue of a different amino acid.

The Asn and/or Gly residue may, for instance, be substituted with a residue of an amino acid selected from the group consisting of A, Q, S, P, T and Y.

More specifically, any of the Asn or Gly residues of the Asn-Gly occupying positions 66-67, 134-135 and/or 375-376 of the SD-521 and Ya protease; and positions 66-67, 134-135, 301-302 and/or 375-376 of the JP170 protease, may be deleted or substituted with a residue of an amino acid selected from the group consisting of A, Q, S, P, T and Y. (positions are indicated in relation to the JP170 protease as indicated in Fig. 1).

Specific variants of JP170 are: N66{\*,A,Q,S,P,T,Y}; G67{\*,A,Q,S,P,T,Y}; N134{\*,A,Q,S,P,T,Y}; G135{\*,A,Q,S,P,T,Y}; N301{\*,A,Q,S,P,T,Y}; G302{\*,A,Q,S,P,T,Y}; N375{\*,A,Q,S,P,T,Y}; and G376{\*,A,Q,S,P,T,Y}; and combinations thereof, such as N66{\*,A,Q,S,P,T,Y}+N134{\*,A,Q,S,P,T,Y}, N66{\*,A,Q,S,P,T,Y}+N301{\*,A,Q,S,P,T,Y}, and

N66{\*,A,Q,S,P,T,Y}+N375{\*,A,Q,S,P,T,Y}, etc.

Specific variants of SD-521 and Ya proteases are: N66{\*,A,Q,S,P,T,Y}; G67{\*,A,Q,S,P,T,Y}; N134{\*,A,Q,S,P,T,Y}; G135{\*,A,Q,S,P,T,Y}; and N375{\*,A,Q,S,P,T,Y}; G376{\*,A,Q,S,P,T,Y}, and combinations thereof as indicated above.

## **Modification of Tyrosine residues**

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In relation to wash performance it has been found that the modification of certain tyrosine residues to phenylalanine provides an improved wash performance. Without being bound by any specific theory, it is believed that titration of these Tyr residues in the alkaline wash liquor has negative effects that are alleviated by replacing the Tyr residues with other residues, especially Phe or Trp, particularly Phe.

In JP170 tyrosine residues may be modified in positions: 20, 54, 118, 137, 147, 194, 225, 247, 249, 334, 379, 388, 411, and 418.

In SD-521 and Ya proteases the tyrosine residues may be modified in positions: 17, 20, 54, 137, 147, 187, 243, 247, 249, 299, 319, 334, 361, 379, 386, 388, 411, and 418.

In relation to JP170 the invention thus relates to the variants: Y17{F,W}, Y20{F,W}, Y54{F,W}, Y137{F,W}, Y147{F,W}, Y187{F,W}, Y243{F,W}, Y247{F,W}, Y249{F,W}, Y299{F,W}, Y319{F,W}, Y334{F,W}, Y361{F,W}, Y379{F,W}, Y386{F,W}, Y411{F,W}, and Y418{F,W}. Corresponding modifications are easily identified in other JP170 type subtilases.

# Modification of tryptophan residues

In order to stabilize the protein it may be advantageous to replace or delete tryptophan residues at the surface of the protein, *e.g.*, as described in US 5,118,623. The tryptophan residues may advantageously be substituted for F, T, Q or G. Thus, in a further embodiment the invention relates to JP170 type subtilase variants comprising one or more of the following substitutions: For the SD-521 and Ya proteases positions 118, 129, 240, 306, 350, and 392; and for the JP170 protease positions 129, 240, 306, 350, and 392.

Thus, the invention relates to a JP170 variant comprising one or more of the following substitutions W129{F,T,Q,G}, W240{F,T,Q,G}, W306{F,T,Q,G}, W350{F,T,Q,G}, and W392{F,T,Q,G}.

#### **Combined modifications**

The present invention also encompasses any of the above mentioned subtilase variants in combination with any other modification to the amino acid sequence thereof. Especially combinations with other modifications known in the art to provide improved properties to the enzyme are envisaged.

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## Methods of preparing JP170 like or BPN' like subtilase variants

The subtilase variants, i.e. the JP170 and BPN' variants of the present invention may be produced by any known method within the art and the present invention also relates to nucleic acid encoding a subtilase variant of the present invention, a DNA construct comprising said nucleic acid and a host cell comprising said nucleic acid sequence.

In general natural occurring proteins may be produced by culturing the organism expressing the protein and subsequently purifying the protein or it may be produced by cloning a nucleic acid, e.g. genomic DNA or cDNA, encoding the protein into an expression vector, introducing said expression vector into a host cell, culturing the host cell and purifying the expressed protein.

Typically protein variants may be produced by site-directed mutagenesis of a parent protein, introduction into expression vector, host cell etc. The parent protein may be cloned from a strain producing the polypeptide or from an expression library, i.e. it may be isolated from genomic DNA or prepared from cDNA, or a combination thereof.

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In general standard procedures for cloning of genes and/or introducing mutations (random and/or site directed) into said genes may be used in order to obtain a parent subtilase, or subtilase or subtilase variant of the invention. For further description of suitable techniques reference is made to Molecular cloning: A laboratory manual (Sambrook et al. (1989), Cold Spring Harbor lab., Cold Spring Harbor, NY; Ausubel, F. M. et al. (eds.)); Current protocols in Molecular Biology (John Wiley and Sons, 1995; Harwood, C. R., and Cutting, S. M. (eds.)); Molecular Biological Methods for Bacillus (John Wiley and Sons, 1990); DNA Cloning: A Practical Approach, Volumes I and II (D.N. Glover ed. 1985); Oligonucleotide Synthesis (M.J. Gait ed. 1984); Nucleic Acid Hybridization (B.D. Hames & S.J. Higgins eds (1985)); Transcription And Translation (B.D. Hames & S.J. Higgins, eds. (1984)); Animal Cell Culture (R.I. Freshney, ed. (1986)); Immobilized Cells And Enzymes (IRL Press, (1986)); A Practical Guide To Molecular Cloning (B. Perbal, (1984)) and WO 96/34946.

Further, variants could be constructed by:

### Random Mutagenesis

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Random mutagenesis is suitably performed either as localized or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleotide at the positions that are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide can be incorporated into the DNA encoding the subtilase enzyme by any published technique, using, e.g., PCR, LCR or any DNA polymerase and ligase as deemed appropriate.

Preferably, the doping is carried out using "constant random doping", in which the percentage of wild-type and modification in each position is predefined. Furthermore, the doping may be directed toward a preference for the introduction of certain nucleotides, and thereby a preference for the introduction of one or more specific amino acid residues. The doping may be made, e.g., so as to allow for the introduction of 90% wild type and 10% modifications in each position. An additional consideration in the choice of a doping scheme is based on genetic as well as protein-structural constraints. The doping scheme may be made by using the DOPE program which, *inter alia*, ensures that introduction of stop codons is avoided (L.J. Jensen et al. *Nucleic Acid Research*, 26, 697-702 (1998).

When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent subtilase enzyme is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., *Technique*, 1, 1989, pp. 11-15).

The DNA sequence to be mutagenized may conveniently be present in a genomic or cDNA library prepared from an organism expressing the parent subtilase. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenising agent. The DNA to be mutagenized may also be present in a host cell either by being integrated in the genome of said cell or by being present on a vector harbored in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

In some cases it may be convenient to amplify the mutated DNA sequence prior to

performing the expression step b) or the screening step c). Such amplification may be performed in accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

# Localised random mutagenesis

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The random mutagenesis may be advantageously localised to a part of the parent subtilase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

The localised or region-specific, random mutagenesis is conveniently performed by use of PCR generated mutagenesis techniques as described above or any other suitable technique known in the art. Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g., by insertion into a suitable vector, and said part may be subsequently subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

# General method for random mutagenesis by use of the DOPE program

The random mutagenesis may be carried out by the following steps:

- Select regions of interest for modification in the parent enzyme
- 2. Decide on mutation sites and non-mutated sites in the selected region
- 3. Decide on which kind of mutations should be carried out, e.g. with respect to the desired stability and/or performance of the variant to be constructed
- 4. Select structurally reasonable mutations
- 5. Adjust the residues selected by step 3 with regard to step 4.
- 30 6. Analyse by use of a suitable dope algorithm the nucleotide distribution.
  - 7. If necessary, adjust the wanted residues to genetic code realism, e.g. taking into account constraints resulting from the genetic code, e.g. in order to avoid introduction of stop codons; the skilled person will be aware that some codon combinations can-

not be used in practice and will need to be adapted

- 8. Make primers
- 9. Perform random mutagenesis by use of the primers
- 10. Select resulting subtilase variants by screening for the desired improved properties.

Suitable dope algorithms for use in step 6 are well known in the art. One such algorithm is described by Tomandl, D. et al., 1997, Journal of Computer-Aided Molecular Design 11:29-38. Another algorithm is DOPE (Jensen, LJ, Andersen, KV, Svendsen, A, and Kretzschmar, T (1998) Nucleic Acids Research 26:697-702).

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#### Expression vectors

A recombinant expression vector comprising a nucleic acid sequence encoding a subtilase variant of the invention may be any vector that may conveniently be subjected to recombinant DNA procedures and which may bring about the expression of the nucleic acid sequence.

The choice of vector will often depend on the host cell into which it is to be introduced. Examples of a suitable vector include a linear or closed circular plasmid or a virus. The vector may be an autonomously replicating vector, i.e., a vector which exists as an extra-chromosomal entity, the replication of which is independent of chromosomal replication, e.g., a plasmid, an extra-chromosomal element, a mini chromosome, or an artificial chromosome. The vector may contain any means for assuring self-replication. Examples of bacterial origins of replication are the origins of replication of plasmids pBR322, pUC19, pACYC177, pACYC184, pUB110, pE194, pTA1060, and pAMß1. Examples of origin of replications for use in a yeast host cell are the 2 micron origin of replication, the combination of CEN6 and ARS4, and the combination of CEN3 and ARS1. The origin of replication may be one having a mutation which makes it function as temperature-sensitive in the host cell (see, e.g., Ehrlich, 1978, Proceedings of the National Academy of Sciences USA 75:1433).

Alternatively, the vector may be one which, when introduced into the host cell, is integrated into the genome and replicated together with the chromosome(s) into which it has been integrated. Vectors which are integrated into the genome of the host cell may contain any nucleic acid sequence enabling integration into the genome, in particular it may contain nucleic acid sequences facilitating integration into the genome by homologous or non-homologous recombination. The vector system may be a single vector, e.g. plasmid or vi-

rus, or two or more vectors, e.g. plasmids or virus', which together contain the total DNA to be introduced into the genome of the host cell, or a transposon.

The vector may in particular be an expression vector in which the DNA sequence encoding the subtilase variant of the invention is operably linked to additional segments or control sequences required for transcription of the DNA. The term, "operably linked" indicates that the segments are arranged so that they function in concert for their intended purposes, e.g. transcription initiates in a promoter and proceeds through the DNA sequence encoding the subtilase variant. Additional segments or control sequences include a promoter, a leader, a polyadenylation sequence, a propeptide sequence, a signal sequence and a transcription terminator. At a minimum the control sequences include a promoter and transcriptional and translational stop signals.

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The promoter may be any DNA sequence that shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell.

Examples of suitable promoters for use in bacterial host cells include the promoter of the *Bacillus subtilis* levansucrase gene (sacB), the *Bacillus stearothermophilus* maltogenic amylase gene (amyM), the *Bacillus licheniformis* alpha-amylase gene (amyL), the *Bacillus amyloliquefaciens* alpha-amylase gene (amyQ), the *Bacillus subtilis* alkaline protease gene, or the *Bacillus pumilus* xylosidase gene, the *Bacillus amyloliquefaciens* BAN amylase gene, the *Bacillus licheniformis* penicillinase gene (penP), the *Bacillus subtilis* xylA and xylB genes, and the prokaryotic beta-lactamase gene (Villa-Kamaroff et al., 1978, Proceedings of the National Academy of Sciences USA 75:3727-3731). Other examples include the phage Lambda P<sub>R</sub> or P<sub>L</sub> promoters or the E. coli lac, trp or tac promoters or the Streptomyces coelicolor agarase gene (dagA). Further promoters are described in "Useful proteins from recombinant bacteria" in Scientific American, 1980, 242:74-94; and in Sambrook et al., 1989, supra.

Examples of suitable promoters for use in a filamentous fungal host cell are promoters obtained from the genes encoding *Aspergillus oryzae* TAKA amylase, *Rhizomucor miehei* aspartic proteinase, *Aspergillus niger* neutral alpha-amylase, *Aspergillus niger* acid stable alpha-amylase, *Aspergillus niger* or *Aspergillus awamori* glucoamylase (glaA), *Rhizomucor miehei* lipase, *Aspergillus oryzae* alkaline protease, *Aspergillus oryzae* triose phosphate isomerase, *Aspergillus nidulans* acetamidase, *Fusarium oxysporum* trypsin-like protease (as described in U.S. Patent No. 4,288,627, which is incorporated herein by refer-

ence), and hybrids thereof. Particularly preferred promoters for use in filamentous fungal host cells are the TAKA amylase, NA2-tpi (a hybrid of the promoters from the genes encoding *Aspergillus niger* neutral (-amylase and *Aspergillus oryzae* triose phosphate isomerase), and glaA promoters. Further suitable promoters for use in filamentous fungus host cells are the ADH3 promoter (McKnight et al., The EMBO J. 4 (1985), 2093 - 2099) or the tpiA promoter.

Examples of suitable promoters for use in yeast host cells include promoters from yeast glycolytic genes (Hitzeman et al., J. Biol. Chem. 255 (1980), 12073 - 12080; Alber and Kawasaki, J. Mol. Appl. Gen. 1 (1982), 419 - 434) or alcohol dehydrogenase genes (Young et al., in Genetic Engineering of Microorganisms for Chemicals (Hollaender et al, eds.), Plenum Press, New York, 1982), or the TPI1 (US 4,599,311) or ADH2-4c (Russell et al., Nature 304 (1983), 652 - 654) promoters.

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Further useful promoters are obtained from the *Saccharomyces cerevisiae* enolase (ENO-1) gene, the *Saccharomyces cerevisiae* galactokinase gene (GAL1), the *Saccharomyces cerevisiae* alcohol dehydrogenase/glyceraldehyde-3-phosphate dehydrogenase genes (ADH2/GAP), and the *Saccharomyces cerevisiae* 3-phosphoglycerate kinase gene. Other useful promoters for yeast host cells are described by Romanos et al., 1992, Yeast 8:423-488. In a mammalian host cell, useful promoters include viral promoters such as those from Simian Virus 40 (SV40), Rous sarcoma virus (RSV), adenovirus, and bovine papilloma virus (BPV).

Examples of suitable promoters for use in mammalian cells are the SV40 promoter (Subramani et al., Mol. Cell Biol. 1 (1981), 854 -864), the MT-1 (metallothionein gene) promoter (Palmiter et al., Science 222 (1983), 809 - 814) or the adenovirus 2 major late promoter.

An example of a suitable promoter for use in insect cells is the polyhedrin promoter (US 4,745,051; Vasuvedan et al., FEBS Lett. 311, (1992) 7 - 11), the P10 promoter (J.M. Vlak et al., J. Gen. Virology 69, 1988, pp. 765-776), the Autographa californica polyhedrosis virus basic protein promoter (EP 397 485), the baculovirus immediate early gene 1 promoter (US 5,155,037; US 5,162,222), or the baculovirus 39K delayed-early gene promoter (US 5,155,037; US 5,162,222).

The DNA sequence encoding a subtilase variant of the invention may also, if necessary, be operably connected to a suitable terminator.

The recombinant vector of the invention may further comprise a DNA sequence ena-

enabling the vector to replicate in the host cell in guestion.

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The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, or a gene encoding resistance to e.g. antibiotics like ampicillin, kanamycin, chloramphenicol, erythromycin, tetracycline, spectinomycine, neomycin, hygromycin, methotrexate, or resistance to heavy metals, virus or herbicides, or which provides for prototrophy or auxotrophs. Examples of bacterial selectable markers are the dal genes from Bacillus subtilis or Bacillus licheniformis, resistance. A frequently used mammalian marker is the dihydrofolate reductase gene (DHFR). Suitable markers for yeast host cells are ADE2, HIS3, LEU2, LYS2, MET3, TRP1, and URA3. A selectable marker for use in a filamentous fungal host cell may be selected from the group including, but not limited to, amdS (acetamidase), argB (ornithine carbamoyltransferase), bar (phosphinothricin acetyltransferase), hygB (hygromycin phosphotransferase), niaD (nitrate reductase), pyrG (orotidine-5'-phosphate decarboxylase), sC (sulfate adenyltransferase), trpC (anthranilate synthase), and glufosinate resistance markers, as well as equivalents from other species. Particularly, for use in an Aspergillus cell are the amdS and pyrG markers of Aspergillus nidulans or Aspergillus oryzae and the bar marker of Streptomyces hygroscopicus. Furthermore, selection may be accomplished by co-transformation, e.g., as described in WO 91/17243, where the selectable marker is on a separate vector.

To direct a subtilase variant of the present invention into the secretory pathway of the host cells, a secretory signal sequence (also known as a leader sequence, prepro sequence or pre sequence) may be provided in the recombinant vector. The secretory signal sequence is joined to the DNA sequence encoding the enzyme in the correct reading frame. Secretory signal sequences are commonly positioned 5' to the DNA sequence encoding the enzyme. The secretory signal sequence may be that normally associated with the enzyme or may be from a gene encoding another secreted protein.

The procedures used to ligate the DNA sequences coding for the present enzyme, the promoter and optionally the terminator and/or secretory signal sequence, respectively, or to assemble these sequences by suitable PCR amplification schemes, and to insert them into suitable vectors containing the information necessary for replication or integration, are well known to persons skilled in the art (cf., for instance, Sambrook et al.).

More than one copy of a nucleic acid sequence encoding an enzyme of the present invention may be inserted into the host cell to amplify expression of the nucleic acid sequence. Stable amplification of the nucleic acid sequence can be obtained by integrating at

least one additional copy of the sequence into the host cell genome using methods well known in the art and selecting for transformants.

The nucleic acid constructs of the present invention may also comprise one or more nucleic acid sequences which encode one or more factors that are advantageous in the expression of the polypeptide, e.g., an activator (e.g., a trans-acting factor), a chaperone, and a processing protease. Any factor that is functional in the host cell of choice may be used in the present invention. The nucleic acids encoding one or more of these factors are not necessarily in tandem with the nucleic acid sequence encoding the polypeptide.

#### Host cells

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The DNA sequence encoding a subtilase variant of the present invention may be either homologous or heterologous to the host cell into which it is introduced. If homologous to the host cell, i.e. produced by the host cell in nature, it will typically be operably connected to another promoter sequence or, if applicable, another secretory signal sequence and/or terminator sequence than in its natural environment. The term "homologous" is intended to include a DNA sequence encoding an enzyme native to the host organism in question. The term "heterologous" is intended to include a DNA sequence not expressed by the host cell in nature. Thus, the DNA sequence may be from another organism, or it may be a synthetic sequence.

The host cell into which the DNA construct or the recombinant vector of the invention is introduced may be any cell that is capable of producing the present subtilase variants, such as prokaryotes, e.g. bacteria or eukaryotes, such as fungal cells, e.g. yeasts or filamentous fungi, insect cells, plant cells or mammalian cells.

Examples of bacterial host cells which, on cultivation, are capable of producing the subtilase variants of the invention are gram-positive bacteria such as strains of *Bacillus*, e.g. strains of *B. subtilis*, *B. licheniformis*, *B. lentus*, *B. brevis*, *B. stearothermophilus*, *B. alkalophilus*, *B. amyloliquefaciens*, *B. coagulans*, *B. circulans*, *B. lautus*, *B. megaterium* or *B. thuringiensis*, or strains of *Streptomyces*, such as *S. lividans* or *S. murinus*, or gram-negative bacteria such as *Escherichia coli* or *Pseudomonas sp*.

The transformation of the bacteria may be effected by protoplast transformation, electroporation, conjugation, or by using competent cells in a manner known per se (cf. Sambrook et al., supra).

When expressing the subtilase variant in bacteria such as E. coli, the enzyme may

be retained in the cytoplasm, typically as insoluble granules (known as inclusion bodies), or it may be directed to the periplasmic space by a bacterial secretion sequence. In the former case, the cells are lysed and the granules are recovered and denatured after which the enzyme is refolded by diluting the denaturing agent. In the latter case, the enzyme may be recovered from the periplasmic space by disrupting the cells, e.g. by sonication or osmotic shock, to release the contents of the periplasmic space and recovering the enzyme.

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When expressing the subtilase variant in gram-positive bacteria such as *Bacillus* or *Streptomyces* strains, the enzyme may be retained in the cytoplasm, or it may be directed to the extracellular medium by a bacterial secretion sequence. In the latter case, the enzyme may be recovered from the medium as described below.

Examples of host yeast cells include cells of a species of Candida, Kluyveromyces, Saccharomyces, Schizosaccharomyces, Pichia, Hansehula, or Yarrowia. In a particular embodiment, the yeast host cell is a Saccharomyces carlsbergensis, Saccharomyces cerevisiae, Saccharomyces diastaticus, Saccharomyces douglasii, Saccharomyces kluyveri, Saccharomyces norbensis or Saccharomyces oviformis cell. Other useful yeast host cells are a Kluyveromyces lactis, Kluyveromyces fragilis, Hansehula polymorpha, Pichia pastoris, Yarrowia lipolytica, Schizosaccharomyces pombe, Ustilgo maylis, Candida maltose, Pichia quillermondii and Pichia methanolio cell (cf. Gleeson et al., J. Gen. Microbiol. 132, 1986, pp. 3459-3465; US 4,882,279 and US 4,879,231). Since the classification of yeast may change in the future, for the purposes of this invention, yeast shall be defined as described in Biology and Activities of Yeast (Skinner, F.A., Passmore, S.M., and Davenport, R.R., eds, Soc. App. Bacteriol. Symposium Series No. 9, 1980. The biology of yeast and manipulation of yeast genetics are well known in the art (see, e.g., Biochemistry and Genetics of Yeast, Bacil, M., Horecker, B.J., and Stopani, A.O.M., editors, 2nd edition, 1987; The Yeasts, Rose, A.H., and Harrison, J.S., editors, 2nd edition, 1987; and The Molecular Biology of the Yeast Saccharomyces, Strathern et al., editors, 1981). Yeast may be transformed using the procedures described by Becker and Guarente, In Abelson, J.N. and Simon, M.I., editors, Guide to Yeast Genetics and Molecular Biology, Methods in Enzymology, Volume 194, pp. 182-187, Academic Press, Inc., New York; Ito et al., 1983, Journal of Bacteriology 153:163; and Hinnen et al., 1978, Proceedings of the National Academy of Sciences USA 75:1920.

Examples of filamentous fungal cells include filamentous forms of the subdivision Eumycota and Oomycota (as defined by Hawksworth et al., 1995, supra), in particular it may of the a cell of a species of *Acremonium*, such as *A. chrysogenum*, *Aspergillus*, such as A. awamori, A. foetidus, A. japonicus, A. niger, A. nidulans or A. oryzae, Fusarium, such as F. bactridioides, F. cerealis, F. crookwellense, F. culmorum, F. graminearum, F. graminum, F. heterosporum, F. negundi, F. reticulatum, F. roseum, F. sambucinum, F. sarcochroum, F. sulphureum, F. trichothecioides or F. oxysporum, Humicola, such as H. insolens or H. lanuginose, Mucor, such as M. miehei, Myceliophthora, such as M. thermophilum, Neurospora, such as N. crassa, Penicillium, such as P. purpurogenum, Thielavia, such as T. terrestris, Tolypocladium, or Trichoderma, such as T. harzianum, T. koningii, T. longibrachiatum, T. reesei or T. viride, or a teleomorph or synonym thereof. The use of Aspergillus spp. for the expression of proteins is described in, e.g., EP 272 277, EP 230 023.

Examples of insect cells include a *Lepidoptera* cell line, such as *Spodoptera* frugiperda cells or *Trichoplusia ni* cells (cf. US 5,077,214). Culture conditions may suitably be as described in WO 89/01029 or WO 89/01028. Transformation of insect cells and production of heterologous polypeptides therein may be performed as described in US 4,745,051; US 4, 775, 624; US 4,879,236; US 5,155,037; US 5,162,222; EP 397,485).

Examples of mammalian cells include Chinese hamster ovary (CHO) cells, HeLa cells, baby hamster kidney (BHK) cells, COS cells, or any number of other immortalized cell lines available, e.g., from the American Type Culture Collection. Methods of transfecting mammalian cells and expressing DNA sequences introduced in the cells are described in e.g. Kaufman and Sharp, J. Mol. Biol. 159 (1982), 601 - 621; Southern and Berg, J. Mol. Appl. Genet. 1 (1982), 327 - 341; Loyter et al., Proc. Natl. Acad. Sci. USA 79 (1982), 422 - 426; Wigler et al., Cell 14 (1978), 725; Corsaro and Pearson, Somatic Cell Genetics 7 (1981), 603, Ausubel et al., Current Protocols in Molecular Biology, John Wiley and Sons, Inc., N.Y., 1987, Hawley-Nelson et al., Focus 15 (1993), 73; Ciccarone et al., Focus 15 (1993), 80; Graham and van der Eb, Virology 52 (1973), 456; and Neumann et al., EMBO J. 1 (1982), 841 - 845. Mammalian cells may be transfected by direct uptake using the calcium phosphate precipitation method of Graham and Van der Eb (1978, Virology 52:546).

### Methods for expression and isolation of proteins

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To express an enzyme of the present invention the above mentioned host cells transformed or transfected with a vector comprising a nucleic acid sequence encoding an enzyme of the present invention are typically cultured in a suitable nutrient medium under conditions permitting the production of the desired molecules, after which these are recovered from the cells, or the culture broth.

The medium used to culture the host cells may be any conventional medium suitable for growing the host cells, such as minimal or complex media containing appropriate supplements. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. in catalogues of the American Type Culture Collection). The media may be prepared using procedures known in the art (see, e.g., references for bacteria and yeast; Bennett, J.W. and LaSure, L., editors, More Gene Manipulations in Fungi, Academic Press, CA, 1991).

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If the enzymes of the present invention are secreted into the nutrient medium, they may be recovered directly from the medium. If they are not secreted, they may be recovered from cell lysates. The enzymes of the present invention may be recovered from the culture medium by conventional procedures including separating the host cells from the medium by centrifugation or filtration, precipitating the proteinaceous components of the supernatant or filtrate by means of a salt, e.g. ammonium sulphate, purification by a variety of chromatographic procedures, e.g. ion exchange chromatography, gelfiltration chromatography, affinity chromatography, or the like, dependent on the enzyme in question.

The enzymes of the invention may be detected using methods known in the art that are specific for these proteins. These detection methods include use of specific antibodies, formation of a product, or disappearance of a substrate. For example, an enzyme assay may be used to determine the activity of the molecule. Procedures for determining various kinds of activity are known in the art.

The enzymes of the present invention may be purified by a variety of procedures known in the art including, but not limited to, chromatography (e.g., ion exchange, affinity, hydrophobic, chromatofocusing, and size exclusion), electrophoretic procedures (e.g., preparative isoelectric focusing (IEF), differential solubility (e.g., ammonium sulfate precipitation), or extraction (see, e.g., Protein Purification, J-C Janson and Lars Ryden, editors, VCH Publishers, New York, 1989).

When an expression vector comprising a DNA sequence encoding an enzyme of the present invention is transformed/transfected into a heterologous host cell it is possible to enable heterologous recombinant production of the enzyme. An advantage of using a heterologous host cell is that it is possible to make a highly purified enzyme composition, characterized in being free from homologous impurities, which are often present when a protein or peptide is expressed in a homologous host cell. In this context homologous impurities mean any impurity (e.g. other polypeptides than the enzyme of the invention) which origi-

nates from the homologous cell where the enzyme of the invention is originally obtained from.

#### **DETERGENT APPLICATIONS**

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The enzyme of the invention may be added to and thus become a component of a detergent composition.

The detergent composition of the invention may for example be formulated as a hand or machine laundry detergent composition including a laundry additive composition suitable for pre-treatment of stained fabrics and a rinse added fabric softener composition, or be formulated as a detergent composition for use in general household hard surface cleaning operations, or be formulated for hand or machine dishwashing operations, especially for automatic dish washing (ADW).

In a specific aspect, the invention provides a detergent additive comprising the enzyme of the invention. The detergent additive as well as the detergent composition may comprise one or more other enzymes such as a protease, a lipase, a cutinase, an amylase, a carbohydrase, a cellulase, a pectinase, a mannanase, an arabinase, a galactanase, a xylanase, an oxidase, e.g., a laccase, and/or a peroxidase.

In general the properties of the chosen enzyme(s) should be compatible with the selected detergent, (i.e. pH-optimum, compatibility with other enzymatic and non-enzymatic ingredients, etc.), and the enzyme(s) should be present in effective amounts.

<u>Proteases</u>: Suitable proteases include those of animal, vegetable or microbial origin. Microbial origin is preferred. Chemically modified or protein engineered mutants are included. The protease may be a serine protease or a metallo protease, preferably an alkaline microbial protease or a trypsin-like protease. Examples of alkaline proteases are subtilisins, especially those derived from *Bacillus*, e.g., subtilisin Novo, subtilisin Carlsberg, subtilisin 309, subtilisin 147 and subtilisin 168 (described in WO 89/06279). Examples of trypsin-like proteases are trypsin (e.g. of porcine or bovine origin) and the *Fusarium* protease described in WO 89/06270 and WO 94/25583.

Examples of useful proteases are the variants described in WO 92/19729, WO 98/20115, WO 98/20116, and WO 98/34946, especially the variants with substitutions in one or more of the following positions: 27, 36, 57, 76, 87, 97, 101, 104, 120, 123, 167, 170, 194, 206, 218, 222, 224, 235 and 274.

Preferred commercially available protease enzymes include Alcalase<sup>TM</sup>, Savinase<sup>TM</sup>, Primase<sup>TM</sup>, Duralase<sup>TM</sup>, Esperase<sup>TM</sup>, and Kannase<sup>TM</sup> (Novozymes A/S), Maxatase<sup>TM</sup>, Maxacal<sup>TM</sup>, Maxapem<sup>TM</sup>, Properase<sup>TM</sup>, Purafect<sup>TM</sup>, Purafect OxP<sup>TM</sup>, FN2<sup>TM</sup>, and FN3<sup>TM</sup> (Genencor International Inc.).

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<u>Lipases</u>: Suitable lipases include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Examples of useful lipases include lipases from *Humicola* (synonym *Thermomyces*), e.g. from *H. lanuginosa* (*T. lanuginosus*) as described in EP 258 068 and EP 305 216 or from *H. insolens* as described in WO 96/13580, a *Pseudomonas* lipase, e.g. from *P. alcaligenes* or *P. pseudoalcaligenes* (EP 218 272), *P. cepacia* (EP 331 376), *P. stutzeri* (GB 1,372,034), *P. fluorescens*, *Pseudomonas sp.* strain SD 705 (WO 95/06720 and WO 96/27002), *P. wisconsinensis* (WO 96/12012), a *Bacillus* lipase, e.g. from *B. subtilis* (Dartois et al. (1993), Biochemica et Biophysica Acta, 1131, 253-360), *B. stearothermophilus* (JP 64/744992) or *B. pumilus* (WO 91/16422).

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Other examples are lipase variants such as those described in WO 92/05249, WO 94/01541, EP 407 225, EP 260 105, WO 95/35381, WO 96/00292, WO 95/30744, WO 94/25578, WO 95/14783, WO 95/22615, WO 97/04079 and WO 97/07202.

Preferred commercially available lipase enzymes include Lipolase<sup>™</sup> and Lipolase Ultra<sup>™</sup> (Novozymes A/S).

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<u>Amylases:</u> Suitable amylases ( $\alpha$  and/or  $\beta$ ) include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Amylases include, for example,  $\alpha$ -amylases obtained from *Bacillus*, e.g. a special strain of *B. licheniformis*, described in more detail in GB 1,296,839.

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Examples of useful amylases are the variants described in WO 94/02597, WO 94/18314, WO 96/23873, and WO 97/43424, especially the variants with substitutions in one or more of the following positions: 15, 23, 105, 106, 124, 128, 133, 154, 156, 181, 188, 190, 197, 202, 208, 209, 243, 264, 304, 305, 391, 408, and 444.

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Commercially available amylases are Duramyl<sup>TM</sup>, Termamyl<sup>TM</sup>, Fungamyl<sup>TM</sup> and BAN<sup>TM</sup> (Novozymes A/S), Rapidase<sup>TM</sup> and Purastar<sup>TM</sup> (from Genencor International Inc.).

Cellulases: Suitable cellulases include those of bacterial or fungal origin. Chemically modi-

fied or protein engineered mutants are included. Suitable cellulases include cellulases from the genera *Bacillus, Pseudomonas, Humicola, Fusarium, Thielavia, Acremonium,* e.g. the fungal cellulases produced from *Humicola insolens, Myceliophthora thermophila* and *Fusarium oxysporum* disclosed in US 4,435,307, US 5,648,263, US 5,691,178, US 5,776,757 and WO 89/09259.

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Especially suitable cellulases are the alkaline or neutral cellulases having colour care benefits. Examples of such cellulases are cellulases described in EP 0 495 257, EP 0 531 372, WO 96/11262, WO 96/29397, WO 98/08940. Other examples are cellulase variants such as those described in WO 94/07998, EP 0 531 315, US 5,457,046, US 5,686,593, US 5,763,254, WO 95/24471, WO 98/12307 and PCT/DK98/00299.

Commercially available cellulases include Celluzyme<sup>™</sup>, and Carezyme<sup>™</sup> (Novozymes A/S), Clazinase<sup>™</sup>, and Puradax HA<sup>™</sup> (Genencor International Inc.), and KAC-500(B)<sup>™</sup> (Kao Corporation).

<u>Peroxidases/Oxidases:</u> Suitable peroxidases/oxidases include those of plant, bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Examples of useful peroxidases include peroxidases from *Coprinus*, e.g. from *C. cinereus*, and variants thereof as those described in WO 93/24618, WO 95/10602, and WO 98/15257.

Commercially available peroxidases include Guardzyme™ (Novozymes A/S).

The detergent enzyme(s) may be included in a detergent composition by adding separate additives containing one or more enzymes, or by adding a combined additive comprising all of these enzymes. A detergent additive of the invention, i.e. a separate additive or a combined additive, can be formulated e.g. as a granulate, a liquid, a slurry, etc. Preferred detergent additive formulations are granulates, in particular non-dusting granulates, liquids, in particular stabilized liquids, or slurries.

Non-dusting granulates may be produced, e.g., as disclosed in US 4,106,991 and 4,661,452 and may optionally be coated by methods known in the art. Examples of waxy coating materials are poly(ethylene oxide) products (polyethyleneglycol, PEG) with mean molar weights of 1000 to 20000; ethoxylated nonylphenols having from 16 to 50 ethylene oxide units; ethoxylated fatty alcohols in which the alcohol contains from 12 to 20 carbon atoms and in which there are 15 to 80 ethylene oxide units; fatty alcohols; fatty acids; and

mono- and di- and triglycerides of fatty acids. Examples of film-forming coating materials suitable for application by fluid bed techniques are given in GB 1483591. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods. Protected enzymes may be prepared according to the method disclosed in EP 238,216.

The detergent composition of the invention may be in any convenient form, e.g., a bar, a tablet, a powder, a granule, a paste or a liquid. A liquid detergent may be aqueous, typically containing up to 70 % water and 0-30 % organic solvent, or non-aqueous.

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The detergent composition comprises one or more surfactants, which may be non-ionic including semi-polar and/or anionic and/or cationic and/or zwitterionic. The surfactants are typically present at a level of from 0.1% to 60% by weight.

When included therein the detergent will usually contain from about 1% to about 40% of an anionic surfactant such as linear alkylbenzenesulfonate, alpha-olefinsulfonate, alkyl sulfate (fatty alcohol sulfate), alcohol ethoxysulfate, secondary alkanesulfonate, alpha-sulfo fatty acid methyl ester, alkyl- or alkenylsuccinic acid or soap.

When included therein the detergent will usually contain from about 0.2% to about 40% of a non-ionic surfactant such as alcohol ethoxylate, nonylphenol ethoxylate, alkylpolyglycoside, alkyldimethylamineoxide, ethoxylated fatty acid monoethanolamide, fatty acid monoethanolamide, polyhydroxy alkyl fatty acid amide, or N-acyl N-alkyl derivatives of glucosamine ("glucamides").

The detergent may contain 0-65 % of a detergent builder or complexing agent such as zeolite, diphosphate, triphosphate, phosphonate, carbonate, citrate, nitrilotriacetic acid, ethylenediaminetetraacetic acid, diethylenetriaminepentaacetic acid, alkyl- or alkenylsuccinic acid, soluble silicates or layered silicates (e.g. SKS-6 from Hoechst).

The detergent may comprise one or more polymers. Examples are carboxymethylcellulose, poly(vinylpyrrolidone), poly (ethylene glycol), poly(vinyl alcohol), poly(vinylpyridine-N-oxide), poly(vinylimidazole), polycarboxylates such as polyacrylates, maleic/acrylic acid copolymers and lauryl methacrylate/acrylic acid copolymers.

The detergent may contain a bleaching system which may comprise a  $H_2O_2$  source such as perborate or percarbonate which may be combined with a peracid-forming bleach activator such as tetraacetylethylenediamine or nonanoyloxybenzenesulfonate. Alterna-

tively, the bleaching system may comprise peroxyacids of e.g. the amide, imide, or sulfone type.

The enzyme(s) of the detergent composition of the invention may be stabilized using conventional stabilizing agents, e.g., a polyol such as propylene glycol or glycerol, a sugar or sugar alcohol, lactic acid, boric acid, or a boric acid derivative, e.g., an aromatic borate ester, or a phenyl boronic acid derivative such as 4-formylphenyl boronic acid, and the composition may be formulated as described in e.g. WO 92/19709 and WO 92/19708.

The detergent may also contain other conventional detergent ingredients such as e.g. fabric conditioners including clays, foam boosters, suds suppressors, anti-corrosion agents, soil-suspending agents, anti-soil redeposition agents, dyes, bactericides, optical brighteners, hydrotropes, tarnish inhibitors, or perfumes.

In the detergent compositions any enzyme, in particular the enzyme of the invention, may be added in an amount corresponding to 0.01-100 mg of enzyme protein per litre of wash liquor, preferably 0.05-5 mg of enzyme protein per litre of wash liquor, in particular 0.1-1 mg of enzyme protein per litre of wash liquor.

The enzyme of the invention may additionally be incorporated in the detergent formulations disclosed in WO 97/07202 which is hereby incorporated as reference.

### **MATERIALS AND METHODS**

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#### **Textiles**

Standard textile pieces are obtained from EMPA St. Gallen, Lerchfeldstrasse 5, CH-9014 St. Gallen, Switzerland. Especially type EMPA 116 (cotton textile stained with blood, milk and ink) and EMPA 117 (polyester/cotton textile stained with blood, milk and ink). Other atandard textile pieces are obtained from wfk-Cleaning Technology Research Institute, Christenfeld 10, D-41379 Brüggen-Bracht, Germany. Especially type wfk10N (cotton textile stained with egg/pigment), wfk10eggEG (cotton textile stained with egg yolk). Denaturation of wfk10N occurs in an autoclave.

# Method for producing a subtilase variant

The present invention provides a method of producing an isolated enzyme according to the invention, wherein a suitable host cell, which has been transformed with a DNA sequence encoding the enzyme, is cultured under conditions permitting the production of the

enzyme, and the resulting enzyme is recovered from the culture.

When an expression vector comprising a DNA sequence encoding the enzyme is transformed into a heterologous host cell it is possible to enable heterologous recombinant production of the enzyme of the invention. Thereby it is possible to make a highly purified subtilase composition, characterized in being free from homologous impurities.

The medium used to culture the transformed host cells may be any conventional medium suitable for growing the host cells in question. The expressed subtilase may conveniently be secreted into the culture medium and may be recovered there-from by well-known procedures including separating the cells from the medium by centrifugation or filtration, precipitating proteinaceous components of the medium by means of a salt such as ammonium sulfate, followed by chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

#### **EXAMPLE 1**

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### Removal of ion-binding sites from BPN' like subtilases

The below mentioned regions in JP170 and TY145 have been selected for transfer from JP170 and TY145 to Savinase. By use of the molecular methods of preparing subtilase variants as described herein, the Savinase regions (BPN' numbering) are deleted and the JP170 and TY145 regions are inserted instead. Since the Savinase regions are in contact with ion-binding sites, the purpose of the modifications is to remove the ion-binding site from Savinase.

Savinase region A194-L196

JP170 region P209-P217 and

Savinase region L75-L82

TY145 region H83-Y92,

alternatively the modification can be

30 Savinase region A194-L196

JP170 region P209-P217 and

Savinase region L75-L82

JP170 region N79-K83.

## Construction and expression of enzyme variants:

### Site-directed mutagenesis:

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Subtilase JP170 site-directed variants of the invention comprising specific insertions/deletions/substitutions are made by traditional cloning of DNA fragments (Sambrook et al., Molecular Cloning: A Laboratory Manual, 2nd Ed., Cold Spring Harbor, 1989) produced by PCR with oligos containing the desired mutations.

The template plasmid DNA may be pSX222, or an analogue of this containing a variant of subtilisin JP170. Mutations are introduced by oligo directed mutagenesis to the construction of variants.

The subtilisin JP170 variants were transformed into *E. coli*. DNA purified from an over night culture of these transformants is transformed into *B. subtilis* by restriction endonuclease digestion, purification of DNA fragments, ligation, transformation of *B. subtilis*. Transformation of *B. subtilis* is performed as described by Dubnau et al., 1971, J. Mol. Biol. 56, pp. 209-221.

# Site-directed mutagenesis in order to introduce mutations in a specific region:

The overall strategy used to perform site-directed mutagenesis is:

Mutagenic primers (oligonucleotides) are synthesized corresponding to the DNA sequence flanking the sites of mutation, separated by the DNA base pairs defining the insertions / deletions / substitutions.

Subsequently, the resulting mutagenic primers are used in a PCR reaction with the modified plasmid pSX222. The resulting PCR fragment is purified and extended in a second PCR-reaction, the resulting PCR product is purified and extended in a third PCR-reaction before being digested by endonucleases and cloned into the *E. coli - B. subtilis* shuttle vector pSX222. The PCR reactions are performed under normal conditions. The plasmid DNA is transformed into *E. coli* by well-known techniques and one *E. coli* colony is sequenced to confirm the mutation designed.

In order to purify subtilase variants of the invention, the pSX222 expression plasmid comprising a variant of the invention was transformed into a competent *B. subtilis* strain and fermented as described above.

#### **EXAMPLE 2**

# Purification and assessment of enzyme concentration

After fermentation, purification of subtilisin variants is accomplished using Hydrophobic Charge Induction Chromatography (HCIC) and subsequent vacuum filtration.

To capture the enzyme, the HCIC uses a cellulose matrix to which 4-Mercapto-Ethyl-Pyridine (4-MEP) is bound.

Beads of the cellulose matrix sized 80-100 µm are mixed with a media containing yeast and the transformed *B. subtilis* capable of secreting the subtilisin variants and incubated at pH 9.5 in Unifilter® microplates.

As 4-MEP is hydrophobic at pH > 7 and the subtilisin variants are hydrophobic at pH 9.5 a hydrophobic association is made between the secreted enzyme and the 4-MEP on the beads. After incubation the media and cell debris is removed by vacuum filtration while the beads and enzyme are kept on the filter.

To elute the enzyme from the beads the pH is now lowered by washing the filter with an elution buffer (pH 5). Hereby the enzymes part from the beads and can be retrieved from the buffer.

The concentration of the purified subtilisin enzyme variants is assessed by active site titration (AST).

The purified enzyme is incubated with the high affinity inhibitor CI-2A at different concentrations to inhibit a varying amount of the active sites. The protease and inhibitor binds to each other at a 1:1 ratio and accordingly the enzyme concentration can be directly related to the concentration of inhibitor, at which all protease is inactive. To measure the residual protease activity, a substrate (0.6 mM Suc-Ala-Ala-Pro-Phe-pNA in Tris/HCl buffer) is added after the incubation with inhibitor and during the following 4 minutes the development of the degradation product pNA (paranitrophenol) is measured periodically at 405 nm on an Elisa Reader.

Each of the variants listed below were constructed as described above. H243K; S238K; L233T; L233S; L233D; Y247R; H200D; H200A; H200G; E185D; S193Q; S193Y; N390D; G394N; G394F; W240H; G355A; G355S; N316D; N79D; K246R; K83R; H200D+D196N; H243E.

## **EXAMPLE 3**

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Automatic Mechanical Stress Assay (AMSA).

## Description of AMSA-test method:

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Washing experiments are performed in order to asses the wash performance of selected JP170 subtilase variants in detergent compositions. Subtilases of the present application were tested using the Automatic Mechanical Stress Assay (AMSA). With the AMSA, the wash performance of a large quantity of small volume enzyme-detergent solutions can be examined. The AMSA plate has a number of slots for test solutions and a lid firmly squeezing the textile swatch to be washed against all the slot openings. During the washing time, the plate, test solutions, textile and lid are vigorously shaken to bring the test solution in contact with the textile and apply mechanical stress in a regular, periodic oscillating manner. For further description see WO 02/42740 especially the paragraph "Special method embodiments" at page 23-24.

The experiment was conducted under the experimental conditions specified below:

Commercial detergent base	European 3in1 ADW type
Detergent dosage	5 – 5.5 g/L
Test solution volume	160 µL
рН	As is
Wash time	20 minutes
Temperature	50°C
Water hardness	25°dH
Enzyme concentration in test solution	0.25mg/L, 0.5mg/L, 1mg/L, and 2.,5 mg/L for wfk10N; 1mg/L, 2,5mg/L, 4mg/L, and 6mg/L for denatured wfk10N.
Test material	Wfk10N

Water hardness was adjusted to 9°dH by addition of CaCl<sub>2</sub>, MgCl<sub>2</sub>, and NaHCO<sub>3</sub> (Ca<sup>2+</sup>:Mg<sup>2+</sup> = 4:1) to the test system. After washing the textile pieces were flushed in tap water and dried.

The performance of the enzyme variant is measured as the brightness of the colour of the textile samples washed with that specific protease. Brightness can also be expressed

as the intensity of the light reflected from the textile sample when illuminated with white light. When the textile is stained the intensity of the reflected light is lower, than that of a clean textile. Therefore the intensity of the reflected light can be used to measure wash performance of a shuffled protease.

Colour measurements are made with a professional flatbed scanner (PFU DL2400pro, obtainable from: J.M. Thomsen, Dorfgade 2, Dorf, Dronninglund, DK-9330), which is used to capture an image of the washed textile samples. The scans are made with a resolution of 200 dpi and with an output colour dept of 24 bits. In order to get accurate results, the scanner is frequently calibrated with a *Kodak reflective IT8 target*.

To extract a value for the light intensity from the scanned images, a special designed software application is used (*Novozymes Color Vector Analyzer*). The program retrieves the 24 bit pixel values from the image and converts them into values for red, green and blue (RGB). The intensity value (Int) is calculated by adding the RGB values together as vectors and then taking the length of the resulting vector:

$$Int = \sqrt{r^2 + g^2 + b^2}$$

#### Detergents

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Detergents for wash performance tests of the subtilases of the invention can be obtained by purchasing fully formulated commercial detergents at the market and subsequently inactivate the enzymatic components by heat treatment (5 minutes at 85°C in aqueous solution). Moreover a commercial detergent base without enzymes can be purchased directly from the manufacturer. Further a suitable model detergent can be purchased and used for wash performance tests.

The proteases may also be tested in a model detergent composition comprising

	Sodium Tripolyphosphate		23.0%						
	Sodium Citrate Dihydrate		22.3%						
	Sodium Perborate Monohydrate		6.0%						
	Tetraacetyl Ethylendiamine								
5	Sodium Disilicate (noncrystaline)		5.0%						
	Linear Fatty Alcohol Ethoxylate		2.0%						
	(non-ionic surfactant, low foaming	)							
	Maleic acid/Acrylic acid copolymer								
(Sodium salt, 50% active on Sodium Carbonate)									
10	Sodium Carbonate, anhydrous	add to	100%						

Using the above test method in combination with a commercially available detergent the results shown below were obtained. As it appears, the subtilases according to the invention exhibits improved wash performance on egg stains in comparison to the willd type JP170 subtilase with SEQ ID NO:1.

Mutations.	AMSA	"peptide binding loop"
WT JP170	REF	
S193Q	≥	S193Y (Ca-site 1)
S193Y	≥	N390D (Ca-site 2)
N390D	≥	G394N (Ca-site 3)
G394N	>	G394F (Ca-site 3)
G394F	≥	W240H (temperature stability)
W240H	≥	G355A (temperature stability)
G355A	≥	G355S (temperature stability)
K246R	≥	K83R (surface charge distribution)
H200D+D196N	≥	(Ca-site 1)

#### APPENDIX 1

REMARK Complex of JP170 and CI2A inhibitor

REMARK Contents of asymmetric unit subtilisin 2x (433 a.a. x 2)

5 REMARK CI2A inhibitor 2x (a.a. 16 - 83 and 21 - 83)

REMARK small peptide (autodigestion product, a.a. KPSLL, 280 - 284)

REMARK Ca ions 6x, H2O 1115 x

REMARK

10 REMARK Crystallization conditions: (AMB) Hanging drop vapour diffusion

REMARK method where the drop consists of 2  $\mu$ l of 15 - 20 mg.ml-1

REMARK protein concentration, 10 mM Na cacodylate - HCl buffer, pH 6.5

15 REMARK and 1  $\mu$ l of the well solution, 20% w/v PEG 4000, 0.1 M Hepes

REMARK buffer, pH 7.5, 10% v/v isopropanol.

HEADER ---- XX-XXX-XX

XXXX

20 COMPND ---

REMARK 3

REMARK 3 REFINEMENT.

REMARK 3 PROGRAM : REFMAC 5.1.24

REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON

25 REMARK 3

REMARK 3 REFINEMENT TARGET : MAXIMUM LIKELIHOOD

REMARK 3

REMARK 3 DATA USED IN REFINEMENT.

	REMARK	3	RESOLUTION RANGE HIGH (ANGSTROMS) : 1.90
	REMARK	. 3	RESOLUTION RANGE LOW (ANGSTROMS) : 19.96
	REMARK	3	DATA CUTOFF (SIGMA(F)) : NONE
	REMARK	3	COMPLETENESS FOR RANGE (%): 76.65
5	REMARK	3	NUMBER OF REFLECTIONS : 59444
	REMARK	3	
	REMARK	3	FIT TO DATA USED IN REFINEMENT.
	REMARK	3	CROSS-VALIDATION METHOD : NULL
	REMARK	3	FREE R VALUE TEST SET SELECTION : NULL
10	REMARK	3	R VALUE (WORKING + TEST SET) : 0.12256
	REMARK	3	R VALUE (WORKING SET) : 0.12256
	REMARK	3	FREE R VALUE : NULL
	REMARK	3	FREE R VALUE TEST SET SIZE (%) : NULL
	REMARK	3	FREE R VALUE TEST SET COUNT : NULL
15	REMARK	3	
	REMARK	3	FIT IN THE HIGHEST RESOLUTION BIN.
	REMARK	3	TOTAL NUMBER OF BINS USED : 20
	REMARK	3	BIN RESOLUTION RANGE HIGH : 1.901
	REMARK	3	BIN RESOLUTION RANGE LOW : 1.950
20	REMARK	3	REFLECTION IN BIN (WORKING SET): 940
	REMARK	3	BIN R VALUE (WORKING SET): 0.149
	REMARK	3	BIN FREE R VALUE SET COUNT : 0
	REMARK	3	BIN FREE R VALUE : -999.000
	REMARK	3	
25	REMARK	3.	NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT

: 8694 REMARK 3 ALL ATOMS

en tracely.

REMARK 3

REMARK 3 B VALUES.

and programme with a second control of

REMARK 3 FROM WILSON PLOT (A\*\*2) : NULL

REMARK 3 MEAN B VALUE (OVERALL, A\*\*2): 16.479

REMARK 3 OVERALL ANISOTROPIC B VALUE.

REMARK 3 B11 (A\*\*2): 0.05

REMARK 3 B22 (A\*\*2): 0.06

REMARK 3 B33 (A\*\*2): -0.11

REMARK 3 B12 (A\*\*2): 0.00 10

REMARK 3 B13 (A\*\*2): 0.00

REMARK 3 B23 (A\*\*2): 0.00

REMARK 3

REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.

. 3 ESU BASED ON R VALUE 15 REMARK

(A): 0.151

esu based on free R 3 VALUE REMARK

(A): NULL

3 ESU BASED ON MAXIMUM LIKELIHOOD REMARK

20 (A): 0.052

> 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD REMARK

(A\*\*2): 1.828

REMARK 3

REMARK 3 CORRELATION COEFFICIENTS.

25 REMARK 3 CORRELATION COEFFICIENT FO-FC : 0.969

REMARK 3 CORRELATION COEFFICIENT FO-FC FREE: NULL

REMARK 3

	REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES WEIGHT	COUN	T RMS
	REMARK 3 BOND LENGTHS REFINED ATOMS 0.014; 0.021	(A):	7733 ;
5	REMARK 3 BOND LENGTHS OTHERS 0.001; 0.020	(A):	6857 ;
	REMARK 3 BOND ANGLES REFINED ATOMS (DE 1.478; 1.936	GREES):	10540 ;
10	REMARK 3 BOND ANGLES OTHERS (DE 0.815; 3.000	GREES):	15972 ;
	REMARK 3 TORSION ANGLES, PERIOD 1 (1;15.784; 5.000	EGREES):	997
	REMARK 3 CHIRAL-CENTER RESTRAINTS 0.106; 0.200	(A**3):	1197 ;
15	REMARK 3 GENERAL PLANES REFINED ATOMS 0.007; 0.020	(A):	8819 ;
	REMARK 3 GENERAL PLANES OTHERS 0.008; 0.020	(A):	1500 ;
20	REMARK 3 NON-BONDED CONTACTS REFINED ATOM 0.221; 0.300	3 (A):	1552 ;
	REMARK 3 NON-BONDED CONTACTS OTHERS 0.265; 0.300	(A):	8282 ;
	REMARK 3 NON-BONDED TORSION OTHERS 0.089; 0.500	(A):	4417 ;
25	REMARK 3 H-BOND (XY) REFINED ATOMS 0.198; 0.500	(A):	1391 ;
	REMARK 3 POTENTIAL METAL-ION REFINED ATOMS 0.145; 0.500	(A):	25 ;
30	REMARK 3 SYMMETRY VDW REFINED ATOMS 0.129; 0.300	(A):	10 ;
	REMARK 3 SYMMETRY VDW OTHERS 0.268; 0.300	(A):	57 ;

	REMARK 0.272 ;	3 SYMMETRY H-BOND REFINED ATOMS (A): 87; 0.500
	REMARK	3
5	REMARK WEIGHT	3 ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT RMS
	REMARK 0.697 ;	3 MAIN-CHAIN BOND REFINED ATOMS (A**2): 4985; 1.500
	REMARK 1.205 ;	3 MAIN-CHAIN ANGLE REFINED ATOMS (A**2): 8031 ; 2.000
10	REMARK 1.963 ;	3 SIDE-CHAIN BOND REFINED ATOMS (A**2): 2746; 3.000
	REMARK 3.180 ;	3 SIDE-CHAIN ANGLE REFINED ATOMS (A**2): 2509; 4.500
	REMARK	3
15	REMARK	3 NCS RESTRAINTS STATISTICS
	REMARK	3 NUMBER OF NCS GROUPS : NULL
	REMARK	3
	REMARK	3
	REMARK	3 TLS DETAILS
20	REMARK	3 NUMBER OF TLS GROUPS : NULL
	REMARK	3
	REMARK	3
	REMARK	3 BULK SOLVENT MODELLING.
	REMARK	3 METHOD USED : BABINET MODEL WITH MASK
25	REMARK	3 PARAMETERS FOR MASK CALCULATION
	REMARK	3 VDW PROBE RADIUS : 1.40
	REMARK	3 ION PROBE RADIUS : 0.80
	REMARK	3 SHRINKAGE RADIUS : 0.80

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	REMARK	3					·
	REMARK	3 OTH	ER REF	NEMENT RE	MARKS:		
	REMARK	3 НҮГ	ROGENS	HAVE BEEN	ADDED	IN THE RIDING	POSITIONS
	REMARK	3					
5	CISPEP	1 GLY	A 163	PRO A	164		0.00
	CISPEP	2 ALA	A 171	PRO A	172		0.00
•	CISPEP	3 PHE	A 191	GLY A	192		0.00
	CISPEP	4 ASN	A 199	HIS A	200		0.00
	CISPEP	5 GLY	A 208	PRO A	209		0.00
10	CISPEP	6 LYS	A 216	PRO A	217		0.00
	CISPEP	7 ASP	A 236	SER A	237		0.00
	CISPÉP	8 ASP	A 1244	SER A	245	•	0.00
	CISPEP	9 PHE	A 299	PRO A	300		0.00
	CISPEP	10 SER	A 327	THR A	328		0.00
15	CISPEP	11 ALA	A 386	PRO A	387		0.00
	CISPEP	12 GLU	A 414	VAL A	415		0.00
ς	CISPEP	13 GLY	A 423	PRO A	424		0.00
	LINK gap		AS	SN B 316			LYS B 318
20	LINK gap		GI	U B 330			ALA B 332
	LINK gap		LE	EU B 337			LYS B 340
25	LINK gap		GI	U D 330			ALA D 332
	LINK gap		LE	U D 337			LYS D 340
	CISPEP	14 GLY	C 163	PRO C	164		0.00

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	CISPEP	15 AL	A C	171	PRO	С	172				0.00	
	CISPEP	16 PHI	ΞC	191	GLY	С	192		•		0.00	
	CISPEP	17 ASI	1 C	199	HIS	С	200				0.00	
	CISPEP	18 GL	Y C	208	PRO	С	209				0.00	
5	CISPEP	19 LYS	S C	216	PRO	С	217				0.00	
	CISPEP	20 ASI	? C	236	SER	С	237				0.00	
	CISPEP	21 AS	? C	244	SER	С	245				0.00	
	CISPEP	22 PH	E C	299	PRO	С	300				0.00	
	CISPEP	23 SEI	R C	327	THR	С	328				0.00	
10	CISPEP	24 AL	A C	386	PRO	С	387				0.00	
	CISPEP	25 GL	JC	414	VAL	С	415				0.00	
	CISPEP	26 GLY	C	423	PRO	С	424				0.00	
	CRYST1	58.38	37 1	L51.4	:11 6	4.0	54 90.	00 117	.11	90.0	00 P 1 2	1 1
	SCALE1	0.	.0171	L27	0.0000	00	0.0087	68		0.00	000	
15	SCALE2	0.	.0000	000	0.0066	05	0.0000	00		0.000	000	
	SCALE3	0.	.0000	000	0.0000	00	0.0175	39		0.00	000	
	HETATM 14.87	1 A	N N	ASN	^ A 1	•	18	.066	20.8	8 0	-3.996	1.00
20	HETATM 14.47	2 A	C9	ASN	A 1		18	.461	22.0	53	-3.689	1.00
	HETATM 13.33	3 A	010 O	ASN	A 1		19.	.168	22.2	51	-2.661	1.00
	HETATM 14.69	4 A	011 0	ASN	A 1		18.	.108	23.0	29	-4.423	1.00
25	HETATM 14.35	5 A	CA C	ASN	A . 1		. 18.	.499	19.6	35	-3.189	1.00
	HETATM 14.69	6 A	CB C	ASN	A 1		18.	.164	18.3	29	-3.883	1.00

	HETATM 14.08	7 A	CG C	ASN	A	1	16.670	18.063	-4.031	1.00
	HETATM 12.20	8 A	ND2 N	ASN	A	1	16.271	17.100	-5.019	1.00
5	HETATM 14.76	9 A	OD1 O	ASN	A	1	15.768	18.701	-3.206	1.00
	HETATM 14.84	10 A	C C	ASN	A	1 .	19.990	19.659	-2.890	1.00
10	HETATM 14.20	11 A	0 0	ASN	A	1	20.353	19.313	-1.601	1.00
	ATOM 15.84	12 A	N N	ASP	A	2	20.881	19.935	-3.834	1.00
	ATOM 16.82	13 A	CA C	ASP	A	2	22.306	19.835	-3.520	1.00
15	ATOM 17.53	14 A	CB C	ASP	A	2	23.178	20.088	-4.763	1.00
	ATOM 18.18	15 A	CG C	ASP	A	2	23.121	18.947	-5.783	1.00
20	ATOM 20.58	16 A	OD1 O	ASP	A	2	22.652	17.811	-5.493	1.00
	ATOM 22.02	17 A	OD2 O	ASP	A	2	23.544	19.106	-6.931	1.00
	ATOM 17.23	18 A	C C	ASP	A	2	22.712	20.816	-2.413	1.00
25	ATOM 18.17	19 A	0	ASP	A	2	23.671	20.562	-1.703	1.00
	ATOM 17.05	20 A	N N	VAL	<b>A</b> .	3	22.018	21.952	-2.304	1.00
30	ATOM 16.07	21 A	CA C	VAL	A	3	22.374	22.945	-1.311	1.00
^	ATOM 16.60	22 A	CB C	VAL	A	3 .	21.974	24.356	-1.701	1.00

	ATOM 16.25	23 A	CG1 C	VAL	A	3	22.327	25.323	-0.560	1.00
	ATOM 18.81	24 A	CG2 C	VAL	A	3	22.676	24.770	-3.003	1.00
5	ATOM 15.65	25 A	C C	VAL	A	3	21.749	22.565	0.033	1.00
	ATOM 14.41	26 A	0	VAL	A	3	22.431	22.603	1.090	1.00
10	ATOM 13.75	27 A	N N	ALA	A	4	20.497	22.119	-0.012	1.00
	ATOM 14.03	28 A	CA C	ALA	A	4	19.824	21.664	1.196	1.00
	ATOM 13.78	29 A	CB C	ALA	A	4	18.388	21.260	0.881	1.00
15	ATOM 14.28	30 A	C C	ALA	A	4	20.544	20.512	1.876	1.00
	ATOM 14.07	31 A	0	ALA	A	4	20.548	20.406	3.110	1.00
20	ATOM 13.74	32 A	N N	ARG	A	5	21.093	19.617	1.064	1.00
	ATOM 14.95	33 A	CA C	ARG	A	5	21.807	18.445	1.553	1.00
	ATOM 15.61	34 A	CB C	ARG	A	5	22.395	17.709	0.349	1.00
25	ATOM 17.28	35 A	CG C	ARG	A	5	23.452	16.639	0.631	1.00
	ATOM 20.73	36 A	CD C	ARG	A	5	23.873	15.945	-0.672	1.00
30	ATOM 21.95	37 A	NE N	ARG	A	5	24.802	14.852	-0.459	1.00
	ATOM 24.69	38 A	CZ C	ARG	A	5	26.128	14.986	-0.513	1.00

	ATOM 25.62	39 A	NH1 N	ARG	A	5	26.687	16.173	-0.793	1.00
	ATOM 22.96	40 A	NH2 N	ARG	A	5	26.898	13.933	-0.290	1.00
5	ATOM 14.83	41 A	C C	ARG	A	5	22.918	18.840	2.515	1.00
	ATOM 14.86	42 A	0	ARG	A	5	23.135	18.195	3.546	1.00
10	ATOM 15.33	43 A	N N	GLY	A	6	23.641	19.897	2.166	1.00
	ATOM 15.34	44 A	CA C	GLY	A	6	24.677	20.416	3.044	1.00
	ATOM 15.01	45 A	C C	GLY	A	6	24.094	21.124	4.257	1.00
15	ATOM 14.62	46 A	0	GLY	A	6	24.609	20.980	5.362	1.00
	ATOM 14.44	47 A	N N	ILÉ	A	7	23.018	21.879	4.062	1.00
20	ATOM 13.98	48 A	CA C	ILE	A	7	22.411	22.613	5.168	1.00
	ATOM 13.68	49 A	CB C	ILE	A	7	21.266	23.505	4.698	1.00
	ATOM 13.35	50 A	CG1 C	ILE	A	7	21.813	24.676	3.864	1.00
25	ATOM 14.08	51 A	CD1 C	ILE	Α	7	20.794	25.294	2.972	1.00
	ATOM 12.51	52 A	CG2 C	ILE	A	7	20.511	24.072	5.873	1.00
30	ATOM 15.04	53 A	C C	ILE	A	7	21.970	21.664	6.305	1.00
	ATOM 13.35	54 A	0	ILE	A	7	22.273	21.906	7.469	1.00

	ATOM 15.03	55 A	N N	VAI	A	8	21.320	20.558	5.952	1.00
	ATOM 14.89	56 A	CA C	VAL	A	8	20.795	19.628	6.969	1.00
5	ATOM 14.63	57 A	CB C	VAL	A	8	19.419	19.047	6.545	1.00
	ATOM 14.63	58 A	CG1 C	VAL	Α	8	18.472	20.135	6.246	1.00
10	ATOM 15.54	59 A	CG2 C	VAL	A	8	19.526	18.151	5.333	1.00
	ATOM 14.75	60 A	C C	VAL	A	8	21.770	18.511	7.356	1.00
	ATOM 15.23	61 A	0	VAL	A	8	21.438	17.645	8.168	1.00
15	ATOM 14.02	62 A	N N	LYS	A	9	22.983	18.568	6.804	1.00
	ATOM 14.55	⁄63 A	CA C	LYS	A	9	24.061	17.627	7.118	1.00
20	ATOM 15.28	64 A	CB C	LYS	A	9 .	24.374	17.560	8.621	1.00
	ATOM 18.34	65 A	CG C	LYS	A	9	24.553	18.888	9.299	1.00
	ATOM 23.66	66 A	CD C	LYS	A	9	25.757	19.608	8.810	1.00
25	ATOM 28.33	67 A	CE C	LYS	A	9	26.025	20.904	9.618	1.00
	ATOM 31.91	68 A	NZ N	LYS	A	9	27.283	21.559	9.079	1.00
30	ATOM 13.77	69 A	C C	LYS	A	9 ·	23.798	16.226	6.616	1.00
	ATOM 13.96	70 A	0 0	LYS	A	9	24.391	15.256	7.132	1.00

	ATOM 13.98	71 A	N N	ALA A	10	22.979	16.109	5.569	1.00
	ATOM 14.34	72 A	CA C	ALA A	10	22.816	14.830	4.886	1.00
- 5	ATOM 14.47	73 A	CB C	ALA A	10	21.649	14.866	3.848	1.00
	ATOM 14.55	74 A	C C	ALA A	10	24.141	14.437	4.205	1.00
10	ATOM 13.73	75 A	0	ALA A	10	24.409	13.264	4.015	1.00
	ATOM 16.04	76 A	N N	ASP A	11	24.967	15.423	3.860	1.00
	ATOM 17.11	77 A	CA C	ASP A	11	26.278	15.153	3.265	1.00
15	ATOM 17.53	78 A	CB C	ASP A	11	26.899	16.419	2.667	1.00
	ATOM 19.89	79 A	CG C	ASP A	11	27.059	17.547	3.680	1.00
20	ATOM 23.81	80 A	OD1 O	ASP A	11	27.845	18.461	3.375	1.00
	ATOM 20.19	81 A	OD2 O	ASP A	11	26.434	17.635	4.773	1.00
	ATOM 17.57	82 A	C C	ASP A	11	27.219	14.489	4.285	1.00
25	ATOM 17.08	83 A	0	ASP A	11	27.941	13.540	3.947	1.00
	ATOM 17.31	84 A	N N	VAL A	12	27.153	14.945	5.528	1.00
30	ATOM 17.86	85 A	CA C	VAL A			14.338	6.607	1.00
	ATOM 18.12	86 A	CB C	VAL A	12	27.850	15.193	7.893	1.00

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	ATOM 18.00	87 A	CG1 C	VAL	Α	12	28.577	14.533	9.081	1.00
	ATOM 19.36	88 A	CG2 C	VAL	A	12	28.385	16.633	7.631	1.00
5	ATOM 18.14	89 A	C C	VAL	A	12	27.428	12.898	6.835	1.00
	ATOM 18.38	90 A	0	VAL	A	12	28.233	11.956	6.925	1.00
10	ATOM 17.13	91 A	N N	ALA	A	13	26.117	12.696	6.870	1.00
	ATOM 17.08	92 A	CA C	ALA	A	13	25.572	11.353	7.076	1.00
	ATOM 17.00	93 A	CB C	ALA	A	13	24.070	11.400	7.101	1.00
1 <b>5</b>	ATOM 17.57	94 A	C C	ALA	A	13	26.044	10.394	5.981	1.00
	ATOM 16.79	95 A	0	ALA.	A	13	26.472	9.237	6.254	1.00
20	ATOM 17.24	96 A	N N	GLN	A	14	25.934	10.862	4.740	1.00
,	ATOM 17.55	97 A	CA C	GLN	A	14	26.420	10.107	3.582	1.00
	ATOM 17.74	98 A	CB C	GLN	Α	14	25.972	10.825	2.309	1.00
25	ATOM 17.61	99 A		GLN	A	14	24.485	10.673	2.031	1.00
	ATOM	100	CD	GLN	А	14	23.995	11.535	0.887	1.00
00	20.02 ATOM	A .		GLN	A	14	24.788	11.949	0.028	1.00
30	19.60 ATOM 19.07	A 102 A	O NE2 N	GLN	Α	14	22.679	11.789	0.850	1.00
	10.01	4.1					- '			

	ATOM 18.95	103 A	C C	GLN	Α	14	27.949	9.876	3.576	1.00
	ATOM 18.61	104 A	0	GLN	Α	14	28.413	8.729	3.489	1.00
5	ATOM 19.73	105 A	N N	ASN	Α	15	28.730	10.950	3.658	1.00
	ATOM 20.71	106 A	CA C	ASN	A	15	30.185	10.847	3.469	1.00
10	ATOM 20.45	107 A	CB C	ASN	A	15	30.828	12.222	3.244	1.00
	ATOM 22.21	108 A	CG C	ASN	A	15	30.404	12.869	1.959	1.00
	ATOM 25.39	109 A	OD1 O	ASN	A	15	30.098	12.201	0.976	1.00
15	ATOM 23.97	110 A	ND2 N	ASN	A	15	30.390	14.182	1.953	1.00
	ATOM 20.49	111 A	C C	ASN	A	15	30.865	10.185	4.653	1.00
20	ATOM 21.06	112 A	0 0	ASN	Α	15	31.705	9.362	4.469	1.00
	ATOM 21.00	113 A	N N	ASN	A	16	30.495	10.559	5.869	1.00
	ATOM 21.90	114 A	CA C	ASN	A	16	31.148	10.056	7.073	1.00
25	ATOM 22.29	115 A	CB C	ASN	A	16	31.205	11.146	8.136	1.00
	ATOM 26.21	116 A	CG C	ASN	A	16	32.100	12.313	7.751	1.00
30	ATOM 32.71	117 A	OD1 O	ASN	Α	16	32.261	13.260	8.533	1.00
	ATOM 28.57	118 A	ND2 N	ASN	Α	16	32,672	12.268	6.567	1.00

	ATOM 21.95	119 A	C C	ASN	A	16	30.491	8.811	7.692	1.00
	ATOM 22.21	120 A	0	ASN	A	16	31.152	8.065	8.404	1.00
5	ATOM 20.66	121 A	N N	PHE	A	17	29.203	8.578	7.438	1.00
	ATOM 20.24	122 A	CA C	PHE	A	17	28.550	7.392	8.003	1.00
10	ATOM 21.09	123 A	CB C	PHE	A	17	27.415	7.815	8.938	1.00
	ATOM 19.81	124 A	CG C	PHE	Α	17	27.890	8.591	10.134	1.00
	ATOM 24.93	125 A	CD1 C	PHE	Α	17	28.110	7.953	11.348	1.00
15	ATOM 25.33	126 A	CE1 C	PHE	A	17	28.556	8.679	12.459	1.00
	ATOM 23.90	127 A	CZ C	PHE	A	17	28.779	10.016	12.344	1.00
20	ATOM 22.65	128 A	CE2 C	PHE	A	17	28.564	10.651	11.155	1.00
	ATOM 20.02	129 A	CD2 C	PHE	A	17	28.111	9.936	10.052	1.00
	ATOM 19.13	130 A		PHE	A	17	28.061	6.385	6.977	1.00
25	ATOM 20.18	131 A	0 0	PHE	Α	17	27.607	5.336	7.337	1.00
	ATOM 17.84	132 A	N N	GLY	Α	18	28.205	6.685	5.692	1.00
30	ATOM 17.25	133 A	CA C	GLY	Α	18	27.740	5.790	4.640	1.00
	ATOM 16.27	134 A	C C	GLY	A	18	26.220	5.654	4.496	1.00

	ATOM 14.47	135 A	0	GLY	Α	18	25.755	4.667	3.948	1.00
	ATOM 15.24	136 A	N N	LEU	Α	19	25.453	6.651	4.955	1.00
5	ATOM 14.35	137 A	CA C	LEU	A	19	23.980	6.550	5.007	1.00
	ATOM 14.71	138 A	CB C	LEU	Α	19	23.456	7.222	6.270	1.00
10	ATOM 15.58	139 A	CG C	LEU	Α	19	24.013	6.680	7.569	1.00
	ATOM 16.09	140 A	CD1 C	LEU	A	19	23.691	7.633	8.721	1.00
	ATOM 15.86	141 A	CD2 C	LEU	A	19	23.417	5.294	7.793	1.00
15	ATOM 13.82	142 A	C C	LEU	A	19	23.305	7.203	3.820	1.00
	ATOM 13.96	143 A	0 0	LEU	A	19	23.183	8.427	3.775	1.00
20	ATOM 13.81	144 A	N N	TYR	A	20	22.874	6.400	2.854	1.00
	ATOM 14.22	145 A	CA C	TYR	A	20	22.156	6.917	1.714	1.00
	ATOM 14.36	146 A	CB C	TYR	A	20	22.841	6.499	0.386	1.00
25	ATOM 14.09	147 A	CG C	TYR	A	20	24.254	7.034	0.241	1.00
	ATOM 16.48	148 A	CD1 C	TYR	A	20	25.351	6.353	0.792	1.00
30	ATOM 16.91	149 A		TYR	A	20	26.661	6.858	0.663	1.00
	ATOM 18.57	150 A		TYR	A	20	26.859	8.041	-0.034	1.00

	ATOM 21.21	151 A	OH O	TYR	A	20	28.126	8.567	-0.171	1.00
	ATOM 17.45	152 A	CE2 C	TYR	A	20	25.788	8.735	-0.575	1.00
5	ATOM 16.03	153 A	CD2 C	TYR	A	20	24.495	8.217	-0.461	1.00
	ATOM 14.55	154 A	C C	TYR	A	20	20.715	6.433	1.702	1.00
10	ATOM 14.48	155 A	0	TYR	A	20	19.994	6.688	0.723	1.00
	ATOM 14.18	156 A	N N	GLY	A	21	20.297	5.710	2.746	1.00
	ATOM 14.23	157 A	CA C	GLY	A	21	18.947	5.172	2.802	1.00
15	ATOM 14.56	158 A	C C	GLY	A	21	18.749	3.775	2.207	1.00
	ATOM 13.53	159 A	0 0	GLY	A	21	17.611	3.315	2.054	1.00
20	ATOM 14.57	160 A	N N	GLN	A	22	19.838	3.084	1.883	1.00
	ATOM 14.82	161 A	CA C	GLN	A	22	19.722	1.726	1.334	1.00
	ATOM 15.45	162 A	CB C	GLN	A	22	21.095	1.130	0.978	1.00
25	ATOM 17.91	163 A	CG C	GLN	A	22	21.054	-0.151	0.150	1.00
	ATOM 21.79	164 A	CD C	GLN	A	22	20.669	-1.376	0.976	1.00
30	ATOM 22.42	165 A	OE1 O	GLN	Α	22	20.892	-1.414	2.185	1.00
	ATOM 23.11	166 A		GLN	A	22	20.091	-2.379	0.317	1.00

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	ATOM 14.04	167 A	C C	GLN	A	22	19.011	0.831	2.331	1.00
	ATOM 14.39	168 A	0	GLN	Α	22	19.341	0.824	3.516	1.00
5	ATOM 14.26	169 A	N N	GLY	A	23	18.019	0.110	1.836	1.00
	ATOM 14.81	170 A	CA C	GLY	A	23	17.236	-0.859	2.628	1.00
10	ATOM 14.12	171 A	C C	GLY	A	23	15.957	-0.245	3.176	1.00
	ATOM 14.17	172 A	0	GLY	A	23	15.086	-0.948	3.718	1.00
	ATOM 13.54	173 A	N N	GLN	A	24	15.836	1.077	3.057	1.00
15	ATOM 13.27	174 A	CA C	GLN	A	24	14.620	1.773	3.500	1.00
	ATOM 12.64	175 A	CB C	GLN	A	24	14.963	3.090	4.182	1.00
20	ATOM 13.46	176 À	CG C	GLN	Α	24	15.806	2.945	5.450	1.00
	ATOM 15.72	. 177 A	CD C	GLN	A	24	15.150	2.100	6.505	1.00
	ATOM 14.73	178 A	OE1 O	GLN	A	24	14.015	2.387	6.921	1.00
25	ATOM 13.89	179 A	NE2 N	GLN	A	24	15.839	1.026	6.927	1.00
	ATOM 13.19	180 A	C C	GLN	Α	24	13.619	2.022	2.352	1.00
30	ATOM 13.48	181 A	0 0	GLN	A	24	14.005	2.126	1.184	1.00
	ATOM 13.28	182 A	N N	ILE	Α	25	12.324	2.066	2.692	1.00

	ATOM 13.25	183 A	CA C	ILE	A	25	11.280	2.319	1.720	1.00
	ATOM 13.64	184 A	CB C	ILE	A	25	10.404	1.077	1.507	1.00
5	ATOM 15.44	185 A	CG1 C	ILE	A	25	11.267	-0.108	1.030	1.00
	ATOM - 14.73	186 A	CD1 C	ILE	Α	25	10.508	-1.518	0.962	1.00
10	ATOM 13.37	187 A	CG2 C	ILE	A	25	9.303	1.387	0.503	1.00
	ATOM 13.24	188 A	C C	ILE	Α	25	10.447	3.491	2.209	1.00
	ATOM 12.93	189 A	0 0	ILE	A	25	9.884	3.430	3.285	1.00
15	ATOM 12.43	190 A	N N	VAL	A	26	10.438	4.573	1.432	1.00
	ATOM 12.49	191 A	CA C	VAL	A	26	9.656	5.754	1.737	1.00
20	ATOM 12.90	192 A	CB C	VAL	A	26	10.480	7.034	1.585	1.00
	ATOM 11.57	193 A	CG1 C	VAL	A	26	9.671	8.231	2.059	1.00
	ATOM 15.53	194 A	CG2 C	VAL	A	26	11.796	6.928	2.395	1.00
25	ATOM 12.34	195 A	C C	VAL	Α	26	8.465	5.823	0.804	1.00
	ATOM 11.99	196 A	0 0	VAL	Α	26	8.601	5.646	-0.418	1.00
30	ATOM 12.40	197 A	N N	ALA	A	27	7.297	6.044	1.387	1.00
	ATOM 12.49	198 A		ALA	Α	27	6.080	6.289	0.624	1.00

	ATOM 11.39	199 A	CB C	ALA A	. 27	4.846	5.650	1.284	1.00
	ATOM 12.17	200 A	C C	ALA A	27	5.892	7.790	0.546	1.00
5	ATOM 11.39	201 A	0	ALA A	. 27	6.077	8.501	1.526	1.00
	ATOM 11.79	202 A	N N	VAL A	28	5.540	8.243	-0.643	1.00
10	ATOM 11.63	203 A	CA C	VAL A	28	5.168	9.612	-0.910	1.00
	ATOM 11.56	204 A	CB C	VAL A	28	6.054	10.176	-2.003	1.00
	ATOM 12.77	205 A	CG1 C	VAL A	28	5.629	11.625	-2.440	1.00
15	ATOM 11.95	206 A	CG2 C	VAL A	28	7.514	10.079	-1.594	1.00
	ATOM 11.23	207 A	C C	VAL A	28	3.729	9.580	-1.458	1.00
20	ATOM 10.72	208 A	0	VAL A	28	3.470	8.936	-2.459	1.00
	ATOM 10.64	209 A	N N	ALA A	29	2.817	10.294	-0.831	1.00
	ATOM 11.32	210 A	CA C	ALA A	29	1.468	10.435	-1.365	1.00
25	ATOM 11.33	211 A	CB C	ALA A	29	0.441	10.151	-0.298	1.00
	ATOM 11.35	212 A	C C	ALA A	29	1.326	11.842	-1.909	1.00
30	ATOM 11.19	213 A	0 0	ALA A	29	1.404	12.826	-1.161	1.00
	ATOM 11.71	214 A	N N	ASP A	30	1.186	11.937	-3.229	1.00

	ATOM 11.52	215 A	CA C	ASP	A	30	1.266	13.221	-3.917	1.00
	ATOM 11.37	216 A	CB C	ASP	A	30	2.718	13.715	-3.958	1.00
5	ATOM 12.40	217 A	CG C	ASP	A	30	2.802	15.221	-3.852	1.00
	ATOM 12.15	218 A	OD1 O	ASP	A	30	3.385	15.726	-2.871	1.00
10	ATOM 14.39	219 A	OD2 O	ASP	Α	30	2.226	15.973	-4.682	1.00
	ATOM 12.41	220 A	C C	ASP	А	30	0.665	13.113	-5.327	1.00
	ATOM 12.89	221 A	0 0	ASP	Α	30	0.068	12.086	-5.671	1.00
15	ATOM 12.52	222 A	N N	THR	A	31	0.811	14.162	-6.151	1.00
	ATOM 11.62	223 A	CA C	THR	A	31	-0.004	14.263	-7.353	1.00
20	ATOM 11.72	224 A	CB C	THR	Α	31	0.302	15.554	-8.182	1.00
	ATOM 11.44	225 A	OG1 O	THR	A	31	1.709	15.702	-8.423	1.00
	ATOM 11.85		CG2 C	THR	A	31	-0.099	16.789	-7.424	1.00
25	ATOM 12.59	227 A	C C	THR	A	31	0.126	13.041	-8.225	1.00
	ATOM 12.63	228 A	0 0	THR	A	31	-0.868	12.341	-8.494	1.00
30	ATOM 12.03	229 A	N N	GLY	A	32	1.360	12.810	-8.665	1.00
	ATOM 12.81	230 A	CA C	GLY	A	32	1.694	11.788	-9.617	1.00

	ATOM 13.22	231 A	C C	GLY	A	32		3.202	11.763	-9.729	1.00
	ATOM 12.83	232 A	0 0	GLY	A	32		3.885	12.607	-9.135	1.00
5	ATOM 13.41	233 A	N N	LEU	A	33		3.711	10.813	-10.501	1.00
	ATOM 13.86	234 A	CA C	LEU	A	33		5.139	10.622	-10.678	1.00
10	ATOM 13.74	235 A	CB C	LEU	A	33		5.625	9.397	-9.899	1.00
	ATOM 14.12	236 A	CG C	LEU	A	33		7.148	9.234	-9.900	1.00
	ATOM 13.99	237 A	CD1 C	LEU	A	33		7.768	10.273	-8.964	1.00
15	ATOM 15.42	238 A	CD2 C	LEU	A	33	•	7.497	7.818	-9.437	1.00
	ATOM 13.89	239 A	C Ċ	LEU	A	33		5.517	10.505	-12.151	1.00
20	ATOM 14.14	240 A	0	LEU	A	33		5.374	9.444	-12.765	1.00
	ATOM 14.55	241 A	N N	ASP	A	34		6.009	11.612	-12.696	1.00
	ATOM 14.62	242 A		ASP	A <sub>.</sub>	34		6.455	11.701	-14.087	1.00
25	ATOM 14.72	243 A		ASP	A	34		7.899	11.201	-14.224	1.00
	ATOM 15.30	244 A	CG C	ASP	A	34		8.516	11.532	-15.598	1.00
30	ATOM 14.31	245 A		ASP	A	34		9.260	10.694	-16.148	1.00
	ATOM 17.33	246 A	OD2 O	ASP	A	34		8.268	12.602	-16.207	1.00

	ATOM 14.94	247 A	C C	ASP	A	34	5.	470	11.016	-15.060	1.00
	ATOM 15.39	248 A	0	ASP	A	34	4.	. 297	11.415	-15.124	1.00
5	ATOM 16.25	249 A	N N	THR	A	35	5.	927	10.013	-15.816	1.00
	ATOM 16.50	250 A	CA C	THR	A	35	5.	083	9.340	-16.813	1.00
10	ATOM 17.03	251 A	CB C	THR	A	35	5.	912	8.471	-17.786	1.00
	ATOM 17.34	252 A	OG1 O	THR	A	35	6.	700	7.514	-17.051	1.00
	ATOM 17.53	253 A	CG2 C	THR	A	35	6.	922	9.300	-18.593	1.00
15	ATOM 17.26	254 A	C C	THR	A	35	4.	005	8.437	-16.229	1.00
	ATOM 15.49	255 A	0	THR	A	35	3.	111	7.992	-16.946	1.00
20	ATOM 16.59	256 A	N N	GLY	A	36	4.	104	8.104	-14.948	1.00
	ATOM 16.76	257 A	CA C	GLY	Α	36	3.	094	7.259	-14.360	1.00
	ATOM 17.58	258 A	C C	GLY	A	36	3.	308	5.802	-14.660	1.00
25	ATOM 17.55	259 A	0	GLY	A	36	2.	432	4.984	-14.383	1.00
	ATOM 18.31	260 A	N N	ARG	A	37	4.	473	5.465	-15.200	1.00
30	ATOM 19.42	261 A	ÇA C	ARG	A	37.	4.	748	4.091	-15.575	1.00
	ATOM 20.37	262 A	CB C	ARG	A	37	4.	763	3.940	-17.088	1.00

	ATOM 23.71	263 A	CG C	ARG	A	37		3.436	4.298	-17.742	1.00
	ATOM 31.29	264 A	CD C	ARG	A	37		3.283	3.740	-19.140	1.00
5	ATOM 34.29	265 A	NE N	ARG	A	37		4.324	4.233	-20.024	1.00
	ATOM 38.63	266 A	CZ C	ARG	Α	37		4.322	5.434	-20.575	1.00
10	ATOM 39.90	267 A	NH1 N	ARG	A	37		5.331	5.792	-21.361	1.00
	ATOM 40.23	268 A	NH2 N	ARG	A	37		3.305	6.273	-20.362	1.00
	ATOM 19.41	269 A	C C	ARG	Α	37	1	6.072	3.661	-14.998	1.00
15	ATOM 18.12	270 A	.0 0	ARG	Α	3,7		7.065	4.354	-15.150	1.00
	ATOM 19.47	271 A	N N	ASN	Α	38		6.067	2.506	-14.334	1.00
20	ATOM 20.37	272 A	CA C	ASN	A	38		7.254	1.998	-13.703	1.00
	ATOM 20.71	273 A	CB C	ASN	A	38		6.917	1.215	-12.431	1.00
	ATOM 21.12		CG C	ASN	A	38		8.161	0.841	-11.658	1.00
25	ATOM 18.41	275 A	OD1 O	ASN	Α	3.8		9.248	1.337	-11.968	1.00
	ATOM 20.60	276 A	ND2 N	ASN	Α	38		8.023	-0.072	-10.684	1.00
30	ATOM 21.21	277 A	C C	ASN	A	38	•	7.984	1.134	-14.700	1.00
	ATOM 21.03	278 A	0	ASN	A	38		7.918	-0.099	-14.638	1.00

	ATOM 21.69	279 A	N N	ASP	A	39	8.659	1.806	-15.625	1.00
	ATOM 23.22	280 A	CA C	ASP	Α	39	9.363	1.158	-16.718	1.00
5	ATOM 23.19	281 A	CB C	ASP	Α	39	8.405	0.839	-17.882	1.00
	ATOM 24.66	282 A	CG C	ASP	A	39	7.806	2.082	-18.526	1.00
10	ATOM 26.50	283 A	OD1 O	ASP	A	39	6.796	1.945	-19.248	1.00
	ATOM 27.03	284 A	OD2 O	ASP	A	39	8.246	3.239	-18.372	1.00
	ATOM 24.00	285 A	C C	ASP	A	39	10.480	2.075	-17.156	1.00
15	ATOM 23.68	286 A	0	ASP	A	39	10.843	3.004	-16.434	1.00
	ATOM 24.67	287 A	N . N	SER	A	40	11.003	1.832	-18.355	1.00
20	ATOM 24.80	288 A	CA C	SER	A	40	12.166	2.539	-18.847	1.00
	ATOM 25.30	289 A	CB C	SER	A	40	12.777	1.766	-20.041	1.00
	ATOM 25.60	290 A	OG O	SER	A	40	11.925	1.881	-21.163	1.00
25	ATOM 23.51	291 A	C C	SER	A	40	11.815	3.984	-19.228	1.00
	ATOM 24.41	292 A	0 0	SER	A	40	12.687	4.805	-19.375	1.00
30	ATOM 23.14	293 A	N N	SER	A	41	10.532	4.308	-19.317	1.00
	ATOM 21.75	294 A	CA C	SER	A	41	10.097	5.670	-19.621	1.00

	ATOM 22.84	295 A	CB C	SER	A	41	8.620	5.679	-20.037	1.00
•	ATOM 21.43	296 A	OG O	SER	A	41	7.725	5.739	-18.919	1.00
5	ATOM 21.13	297 A	C C	SER	A	41	10.262	6.639	-18.427	1.00
	ATOM 19.88	298 A	0	SER	A	41	10.299	7.863	-18.603	1.00
10	ATOM 19.68	299 A	N N	MET	A	42	10.359	6.079	-17.223	1.00
	ATOM 18.70	300 A	CA C	MET	Α	42	10.381	6.882	-15.996	1.00
	ATOM 18.20	301 A	CB C	MET	A	42	10.295	5.949	-14.782	1.00
15	ATOM 17.87	302 A	CG C	MET	Α	42	10.451	6.626	-13.423	1.00
	ATOM 16.31	303 A	SD S	MET	A	42	9.190	7.804	-13.030	1.00
20	ATOM 15.38	304 A	CE C	MET	A	42	7.658	6.844	-13.134	1.00
	ATOM 17.89	305 A	C C	MET	A	42	11.607	7.779	-15.897	1.00
	ATOM 17.28	306 A	0 0	MET	A	42	12.728	7.390	-16.223	1.00
25	ATOM 17.69	307 A	N N	HIS	A	43	11.381	8.998	-15.421	1.00
	ATOM 17.38	308 A	CA C	HIS	A	43	12.479	9.903	-15.081	1.00
30	ATOM 17.29	309 A	CB C	HIS	Α	43	11.942	11.020	-14.196	1.00
	ATOM 16.73	310 A	CG C	HIS	A	43	12.896	12.155	-13.981	1.00

	ATOM 16.98	311 A	ND1 N	HIS	A	43	12.576	13.456	-14.321	1.00
	ATOM 13.61	312 A	CE1 C	HIS	A	43	13.566	14.257	-13.971	1.00
5	ATOM 17.49	313 A	NE2 N	HIS	A	43	14.521	13.523	-13.426	1.00
	ATOM 13.70	314 A	CD2 C	HIS	Α	43	14.113	12.207	-13.397	1.00
10	ATOM 16.64	315 A	C C	HIS	A	43	13.647	9.209	-14.381	1.00
	ATOM 15.82	316 A	0	HIS	A	43	13.453	8.389	-13.479	1.00
	ATOM 16.35	317 A	N N	GLU	A	44	14.858	9.559	-14.818	1.00
15	ATOM 16.74	318 A	CA C	GLU	Α	44	16.112	8.985	-14.358	1.00
	ATOM 17.71	319 A	CB C	GLU	A	44	17.293	9.763	-14.988	1.00
20	ATOM 18.20	320 A	CG C	GLU	A	44	17.268	11.270	-14.753	1.00
	ATOM 22.20	321 A	CD C	GLU	Α	44	18.445	12.004	-15.418	1.00
	ATOM 20.94	322 A	OE1 O	GLU	A	44	18.997	11.455	-16.397	1.00
25	ATOM 20.93	323 A	OE2 O	GLU	Α	44	18.843	13.110	-14.933	1.00
	ATOM 17.11	324 A	C C	GLU	A	44	16.280	8.982	-12.823	1.00
30	ATOM 17.08	325 A	0 0	GLU	A	44	16.944	8.104	-12.259	1.00
	ATOM 16.39	326 A	N N	ALA	A	45	15.665	9.954	-12.152	1.00

	ATOM 16.01	327 A	CA C	ALA	A	45	15.7	74 10.061	-10.696	, 1.00
	ATOM 15.44	328 A	CB C	ALA	Α	45	15.1	22 11.354	-10.198	1.00
5	ATOM 16.39	329 A	C C	ALA	A	45	15.19	8.864	-9.971	1.00
	ATOM 14.42	330 A	0	ALA	A	45	15.53	8.564	-8.857	1.00
10	ATOM 16.01	331 A	. N N	PHE	A	46	14.18	84 8.218	-10.595	1.00
	ATOM 16.28	332 A	CA C	PHE	A	46	13.41	7.139	-9.971	1.00
	ATOM 16.14	333 A	CB C	PHE	A	46	11.95	7.562	-9.882	1.00
15	ATOM 14.90	334 A	CG <sup>°</sup>	PHE	A	46	11.78	8.959	-9.396	1.00
	ATOM 14.17	335 A	CD1 C	PHE	A	46	12.03	9.275	-8.078	1.00
20	ATOM 13.19	336 A	CE1 C	PHE	A	46	11.89	10.586	-7.628	1.00
	ATOM 14.92	337 A	CZ C	PHE	A	46	11.52	25 11.592	-8.504	1.00
	ATOM 16.01	338 A	CE2 C	PHE	A	46	11.29	11.299	-9.809	1.00
25	ATOM 15.93	339 A	CD2 C	PHE	A	46	11.41	.6 9.971	-10.261	1.00
	ATOM 17.23	340 A	Ċ C	PHE	A	46	13.46	56 5.791	-10.697	1.00
30	ATOM 16.06	341 A	0	PHE	A	46	13.01	.7 4.764	-10.172	1.00
	ATOM 18.87	342 A	N N	ARG	A	47	13.98	5.781	-11.917	1.00

	ATOM 20.32	343 A	CA C	ARG	A	47	13.963	4.566	-12.723	1.00
	ATOM 21.00	344 A	CB C	ARG	A	47	14.659	4.833	-14.062	1.00
5	ATOM 24.13	345 A	CG C	ARG	Α	47	14.309	3.871	-15.173	1.00
	ATOM 28.53	346 A	CD C	ARG	A	47	14.468	4.517	-16.570	1.00
10	ATOM 32.22	347 A	NE N	ARG	A	47	15.803	5.031	-16.813	1.00
	ATOM 34.45	348 A	CZ C	ARG	A	47	16.105	6.229	-17.359	1.00
	ATOM 33.97	349 A	NH1 N	ARG	A	47	15.171	7.109	-17.703	1.00
15	ATOM 33.82	350 A	NH2 N	ARG	A	47	17.384	6.558	-17.527	1.00
	ATOM 20.49	351 A	C C	ARG	Α	47	14.674	3.437	-12.000,	1.00
20	ATOM 21.38	352 A	0	ARG	A	47	15.784	3.619	-11.523	1.00
	ATOM 21.45	353 A	\N N	GLY	A	48	14.032	2.280	-11.898	1.00
	ATOM 21.59		CA C	GLY	A	48	14.642	1.105	-11.274	1.00
25	ATOM 21.98	355 A	C C	GLY	A	48	14.583	1.091	-9.741	1.00
	ATOM 21.74	356 A	0 0	GLY	A	48	15.072	0.145	-9.102	1.00
30 -	ATOM 21.05	357 A	N N	LYS	A	49	13.984	2.117	-9.136	1.00
	ATOM 20.90	358 A	CA C	LYS	A	49	13.950	2.197	-7.662	1.00

	ATOM 22.03	359 A	CB C	LYS	A	49	14.915	3.305	-7.180	1.00
	ATOM 24.83	360 A	CG C	LYS	. <b>A</b>	49	14.366	4.713	-7.161	1.00
5	ATOM 27.45	361 A	CD C	LYS	A	49	15.447	5.815	-6.761	1.00
	ATOM 27.82	362 A	CE C	LYS	A	49	15.957	5.680	-5.358	1.00
10	ATOM 28.25	363 A	NZ N	LYS	A	49	17.024	4.667	-5.220	1.00
	ATOM 19.90	364 A	C C	LYS	A	49	12.523	2.329	-7.077	1.00
	ATOM 19.91	365 A	0 0	LYS	A	49	12.339	2.667	-5.890	1.00
15	ATOM 18.63	366 A	N N	ILE	A	50	11.523	1.999	-7.900	1.00
	ATOM . 17.48	367 A	CA C	ILE	A	50	10.121	2.078	-7.533	1.00
20	ATOM 17.67	368 A	CB C	ILE	A	50	9.284	2.650	-8.695	1.00
	ATOM 17.24	369 A	CG1 C	ILE	A	50	9.738	4.076	-9.050	1.00
	ATOM 17.34	370 A	CD1 C	ILE	Α	50	9.083	4.630	-10.302	1.00
25	ATOM 17.29	371 A	CG2 C	ILE	Α	50	7.807	2.723	-8.319	1.00
	ATOM 17.96	372 A	C C	ILE	A	50	9.562	0.730	-7.090	1.00
30	ATOM 18.69	373 A	0 0	ILE	A	50	9.339	-0.161	-7.909	1.00
	ATOM 17.09	374 A	N N	THR	A	51	9.355	0.583	-5.784	1.00

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	ATOM 17.60	. 375 A	CA C	THR	Α	51	8.73	1 -0.601	-5.218	1.00
	ATOM 18.38	376 A	CB C	THR	A	51	8.70	0 -0.423	-3.690	1.00
5	ATOM 17.39	377 A	OG1 O	THR	A	51	10.03	3 -0.380	-3.205	1.00
	ATOM 17.34	378 A	CG2 C	THR	Α	51	8.05	4 -1.617	-3.014	1.00
10	ATOM 17.50	379 A	C C	THR	A	51	7.30	1 -0.746	-5.646	1.00
	ATOM 18.10	380 . A	0 0	THR	A	51	6.82	7 -1.834	-5.903	1.00
	ATOM 16.93	381 A	N N	ALA	Α	52	6.578	3 0.369	-5.670	1.00
15	ATOM 17.34	382 A	CA C	ALA	A	52	5.179	0.338	-6.052	1.00
	ATOM 17.41	383 A	CB C	ALA	A	52	4.31	4 -0.132	-4.884	1.00
20	ATOM 17.46	384 A	C C	ALA	A	52	4.753	3 1.725	-6.501	1.00
	ATOM 16.50	385 A	0 0	ALA	A	52	5.18	7 2.730	-5.928	1.00
	ATOM 17.19	386 A	N N	LEU	A	53	3.92	1.760	-7.539	1.00
25	ATOM 16.89	387 A	CA C	LEU	A	53	3.369	2.987	-8.081	1.00
	ATOM 16.66	388 A	CB C	LEU	A	53.	4.004	3.309	-9.430	1.00
30	ATOM 16.83	389 A	CG C	LEU	Α	53	3.490	4.525	-10.224	1.00
	ATOM 15.83	390 A	CD1 C	LEU	Α	53	3.523	5.796	-9.401	1.00

	ATOM 17.71	391 A	CD2 C	LEU	A	53	4.303	4.720	-11.476	1.00
	ATOM 17.28	392 A	C C	LEU	Α	53	1.868	2.779	-8.212	1.00
5	ATOM 17.43	393 A	0	LEU	A	53	1.421	2.057	-9.097	1.00
	ATOM 17.28	394 A	N N	TYR	A	54	1.101	3.393	-7.303	1.00
10	ATOM 16.87	395 A	CA C	TYR	A	54	-0.350	3.200	-7.230	1.00
	ATOM 16.88	396 A	CB C	TYR	A	54	-0.774	2.944	-5.789	1.00
	ATOM 15.63	397 A	CG C	TYR	A	54	-0.268	1.679	-5.144	1.00
15	ATOM 15.86	398 A	CD1 C	TYR	A	54	-0.411	0.448	-5.770	1.00
	ATOM 15.12	399 A	CE1 C	TYR	A	54	0.037	-0.698	-5.192	1.00
20	ATOM 15.32	400 A	CZ C	TYR	A	54	0.666	-0.647	-3.946	1.00
	ATOM 14.97	401 A	OH O	TYR	A	54	1.093	-1.815	-3.374	1.00
	ATOM 15.70	402 A	CE2 C	TYR	A	54	0.856	0.558	-3.312	1.00
25	ATOM 15.59	403 A	CD2 C	TYR	A	54	0.384	1.718	-3.908	1.00
	ATOM 17.11	404 A	C C	TYR	A	54	-1.098	4.411	-7.712	1.00
30	ATOM 16.78	405 A	0	TYR	A	54	-0.733	5.546	-7.387	1.00
	ATOM 17.01	406 A	N N	ALA	A.	55	-2.161	4.184	-8.483	1.00

	ATOM 17.49	407 A	CA C	ALA	Α	55	-3.032	5.260	-8.926	1.00
	ATOM 17.43	408 A	CB C	ALA	A	55	-3.355	5.094	-10.437	1.00
5	ATOM 18.26	409 A	C C	ALA	Α	55	-4.323	5.272	-8.100	1.00
	ATOM 19.60	410 A	0	ALA	A	55	-5.174	4.400	-8.269	1.00
10	ATOM 17.69	411 A	N N	LEU	A	56	-4.481	6.267	-7.230	1.00
	ATOM 17.32	412 A	CA C	LEU	A	56	-5.641	6.353	-6.368	1.00
	ATOM 16.99	413 A	CB C	LEU	A	56	-5.224	6.779	-4.965	1.00
15	ATOM 17.97	414 A	CG C	LEU	A	56	-4.452	5.752	-4.129	1.00
	ATOM 20.33	415 A	CD1 C	LEU	Α	56	-3.120	5.532	-4.719	1.00
20	ATOM 19.18	416 A	CD2 C	LEU	A	56	-4.329	6.225	-2.662	1.00
	ATOM 17.28	417 A	C ·	LEU	A	56	-6.662 ·	7.360	-6.867	1.00
	ATOM 17.95	418 A	_	LEU	A	56	-7.839	7.192	-6.653	1.00
25	ATOM 17.26	419 A	N			57	-6.204			
	ATOM 17.53	420 A	С			57	-7.068	9.541	-7.802	1.00
30	ATOM 17.74	421 A	С				-7.662			
	ATOM 17.69	422 A	0	GLY	Α	57	-8.758	9.905	-9.446	1.00

	ATOM 18.54	423 A	N N	ARG	A 5	8	-6.921	8.825	-10.109	1.00
	ATOM 19.44	424 A	CA C	ARG	A 5	8	-7.361	8.659	-11.502	1.00
5	ATOM 18.56	425 A	CB C	ARG	A 5	8	-6.572	9.555	-12.466	1.00
	ATOM 18.16	426 A	CG C	ARG	A 5	8	-6.873	11.036	-12.371	1.00
10	ATOM 17.99	427 A	CD C	ARG	A 5	8	-5.685	11.912	-12.787	1.00
	ATOM 17.16	428 A	NE N	ARG	A 5	8	-4.505	11.593	-11.990	1.00
	ATOM 18.78	429 A	CZ C	ARG	A 5	8	-3.248	11.716	-12.392	1.00
15	ATOM 18.96	430 A	NH1 N	ARG 2	A 58	3	-2.967	12.194	-13.591	1.00
	ATOM 17.60	431 A	NH2 N	ARG 2	A 58	3	-2.253	11.339	-11.584	1.00
20	ATOM 19.97	432 A	C C	ARG .	A 58	8	-7.123	7.240	-11.909	1.00
	ATOM 20.06	433 A	0	ARG .	A 58	3	-6.007	6.754	-11.878	1.00
	ATOM 22.06	434 A	N N	THR Z	A 59	€	-8.183	6.575	-12.324	1.00
25	ATOM 22.88	435 A	CA C	THR A	A 59	)	-8.091	5.180	-12.688	1.00
	ATOM 24.04	436 A	CB C	THR A	A 59	)	-9.479	4.693	-13.142	1.00
30	ATOM 25.24	437 A	OG1 O	THR A	A 59	)	-10.330	4.643	-11.984	1.00
	ATOM 25.24	438 À	CG2 C	THR A	A 59		-9.406	3.250	-13.657	1.00

	ATOM 22.06	439 A	C C	THR	. A	59		-7.009	4.919	-13.733	1.00
	ATOM 22.93	440 A	0	THR	. A	59		-7.020	5.482	-14.835	1.00
5	ATOM 21.27	441 A	N N	ASN	Α	60		-6.074	4.068	-13.332	1.00
	ATOM 21.57	442 A	CA C	ASN	Α	60		-4.939	3.618	-14.124	1.00
10	ATOM 22.51	443 A	CB ·C	ASN	Α	60		-5.400	2.788	-15.326	1.00
	ATOM 24.76	444 A	CG C	ASN	A	60		-5.861	1.401	-14.927	1.00
	ATOM 27.82	445 A	OD1 O	ASN	A	60		-5.546	0.908	-13.835	1.00
15	ATOM 25.97	446 A	ND2 N	ASN	A	60		-6.624	0.773	-15.801	1.00
	ATOM 20.35	447 A	C C	ASN	Α	60		-4.038	4.744	-14.614	1.00
20	ATOM 20.71	448 A	0 0	ASN	Α	60		-3.369	4.589	-15.629	1.00
	ATOM 18.43	449 A	N N	ASN	A	61		-4.023	5.852	-13.897	1.00
	ATOM 18.53	450 A	CA C	ASN	A	61		-3.217	6.996	-14.300	1.00
25	ATOM 17.54	451 A	CB C	ASN	A	61	•	-4.095	8.062	-14.972	1.00
	ATOM 19.62	452 A	CG C	ASN	Α	61		-3.278	9.194	-15.580	1.00
30	ATOM 22.44	453 A		ASN	A	61		-3.832	10.171	-16.141	1.00
	ATOM 15.52	454 A		ASN	Α	61		-1.968	9.081	-15.481	1.00

	ATOM 16.75	455 A	C C	ASN	Α	61	-2.520	7.586	-13.088	1.00
	ATOM 16.00	456 A	0	ASN	Α	61	-3.159	8.213	-12.260	1.00
5	ATOM 16.29	457 A	N N	ALA	. A	62	-1.219	7.357	-12.988	1.00
	ATOM 16.34	458 A	CA C	ALA	A	62	-0.418	7.910	-11.902	1.00
10	ATOM 16.55	459 A	CB C	ALA	A	62	0.310	6.804	-11.183	1.00
	ATOM 16.52	460 A	C C	ALA	A	62	0.584	8.948	-12.405	1.00
	ATOM 15.61	461 A	0	ALA	A	62	1.583	9.221	-11.728	1.00
15	ATOM 15.91	462 A	N N	ASN	A	63	0.344	9.515	-13.593	1.00
	ATOM 15.75	463 A	CA C	ASN	A	63	1.276	10.465	-14.157	1.00
20	ATOM 15.36	464 A	CB C	ASN	Α	63	1.251	10.471	-15.720	1.00
	ATOM 16.00	465 A	CG C	ASN	Α	63	0.043	11.165	-16.307	1.00
	ATOM 14.50	466 A	OD1 O	ASN	A	63	-0.617	11.982	-15.643	1.00
25	ATOM 15.36	467 A	ND2 N	ASN	A	63	-0.274	10.833	-17.584	1.00
	ATOM 15.21	468 A	C C	ASN	A	63	1.115	11.858	-13.518	1.00
30	ATOM 15.63	469 A	0 0	ASN	A	63	0.168	12.108	-12.762	1.00
	ATOM 15.12	470 A	N N	ASP	A	64	2.047	12.753	-13.828	1.00

	ATOM 15.29	471 A	CA C	ASP	Α	64	2.192	14.015	-13.102	1.00
	ATOM 14.59	472 A	CB C	ASP	A	64	3.450	13.990	-12.233	1.00
5	ATOM 15.31	473 A	CG C	ASP	A	64	3.532	15.161	-11.300	1.00
	ATOM 14.15	474 A	OD1 O	ASP	A	64	2.476	15.813	-11.058	1.00
10	ATOM 14.37	475 A	OD2 O	ASP	A	64	4.626	15.516	-10.776	1.00
	ATOM 15.53	476 A	C	ASP	A	64	2.236	15.206	-14.061	1.00
	ATOM 16.54	477 A	0	ASP	A	64	3.315	15.713	-14.423	1.00
15	ATOM 16.18	478 A	N N	PRO	Α	65	1.065	15.644	-14.476	1.00
	ATOM 17.33	479 A	CA C	PRO	A	65	0.950	16.813	-15.343	1.00
20	ATOM 17.19	480 A	CB C	PRO	A	65	-0.509	16.776	-15.807	1.00
	ATOM 17.73	481 A	CG C	PRO	A	65	-1.225	15.953	-14.808	1.00
	ATOM 17.21		CD C	PRO	Α	65	-0.249	15.043	-14.172	1.00
25	ATOM 17.72	483 A	C C	PRO	Α	65	1.228	18.102	-14.607	1.00
	ATOM 17.98	484 A	0	PRO	A	65	1.515	19.081	-15.250	1.00
30	ATOM 18.27	485 A	N N	ASN	A	66	1.150	18.065	-13.279	1.00
	ATOM 19.24	486 A	CA C	ASN .	A	66	1.314	19.217	-12.426	1.00

	ATOM 20.48	487 A	CB C	ASN	A	66		0.536	18.958	-11.111	1.00
	ATOM 22.89	488 A	CG C	ASN	Α	66		0.790	19.993	-10.068	1.00
5	ATOM 23.54	489 A	OD1 O	ASN	Α	66		1.942	20.281	-9.721	1.00
	ATOM 25.20	490 A	ND2 N	ASN	Α	66		-0.287	20.591	-9.566	1.00
10	ATOM 18.71	491 A	C C	ASN	A	66		2.806	19.457	-12.153	1.00
	ATOM 18.84	492 A	0	ASN	A	66		3.314	20.549	-12.353	1.00
	ATOM 17.55	493 A	N N	GLY	A	67		3.500	18.426	-11.698	1.00
15	ATOM 16.38	494 A	CA C	GLY	Α	67		4.917	18.503	-11.406	1.00
	ATOM 15.32	495 A	C C	GLY	A	67		5.234	18.455	-9.916	1.00
20	ATOM 15.11	496 A	0 0	GLY	Α.	67	-	6.383	18.167	-9.542	1.00
	ATOM 13.44	497 A	N N	HIS	A	68		4.230	18.722	-9.075	1.00
	ATOM 12.51	498 A	CA C	HIS .	A	68 -		4.406	18.776	-7.608	1.00
25	ATOM 12.22	499 A	CB B	HIS 2	Ą	68		3.109	19.121	-6.891	0.50
	ATOM 12.48	500 A	CB A	HIS A	A	68		3.048	19.078	-6.930	0.50
30	ATOM 10.61	501 A	CG B	HIS A	A	68		3.266	19.371	-5.417	0.50
	ATOM 10.86	502 A	CG AI	HIS A	Ą	68		3.140	19.398	-5.464	0.50

	ATOM 5.34	503 A	ND1BHIS N	Α	68	2.741	18.522	-4.453	0.50
	ATOM 7.56	504 A	ND1AHIS N	A	68	3.742	18.559	-4.548	0.50
5	ATOM 6.59	505 A	CE1BHIS C	Α	68	3.009	19.016	-3.254	0.50
	ATOM 2.00	506 A	CE1AHIS C	A	68	3.674	19.102	-3.341	0.50
10	- ATOM 7.98	507 A	NE2BHIS N	A	68	3.678	20.158	-3.403	0.50
	ATOM 6.21	508 A	NE2AHIS N	A	68	3.061	20.277	-3.442	0.50
	ATOM 5.10	509 A	CD2BHIS C	A	68	3.845	20.405	-4.745	0.50
15	ATOM 8.79	510 A	CD2AHIS C	A	68	2.697	20.471	-4.756	0.50
	ATOM 12.70	511 A	C HIS	A	68	4.986	17.474	-7.064	1.00
20	ATOM 12.91	512 A	O HIS	A	68	6.025	17.471	-6.401	1.00
	ATOM 13.22	513 A	N GLY	A	69	4.315	16.374	-7.317	1.00
	ATOM 13.52	514 A	CA GLY	Α	69	4.709	15.094	-6.739	1.00
25	ATOM 13.01	515 A	C GLY	A	69	6.039	14.574	-7.181	1.00
	ATOM 13.80	516 - A		A	69	6.751	13.894	-6.418	1.00
30	ATOM 13.25	517 A	N THR	A	70	6.391	14.865	-8.432	1.00
	ATOM 12.89	518 A	CA THR	A	70	7.651	14.425	-8.970	1.00

	ATOM 13.93	519 A	CB THE C	R A	70	7	.688	14.638	-10.507	1.00
	ATOM 14.34	520 A	OG1 THR O	. A	70	6	.592	13.940	-11.116	1.00
5	ATOM 13.50	521 A	CG2 THR C	. A	70	, 8	.895	13.977	-11.110	1.00
	ATOM 12.86	522 A	C THR	A	70	. 8	.769	15.192	-8.309	1.00
10	ATOM 13.63	523 A	O THR	A	70	9.	.816	14.622	-8.013	1.00
	ATOM 12.19	524 A	N HIS	A	71	8 .	.560	16.498	-8.093	1.00
	ATOM 11.80	525 A	CA HIS	Α	71	9.	.580	17.341	-7.486	1.00
15	ATOM 11.41	526 A	CB HIS	A	71	9.	.125	18.796	-7.555	1.00
	ATOM 11.89	527 A	CG BHIS	A	71	10.	185	19.784	-7.212	0.50
20	ATOM 9.73	528 A	CG AHIS	A	71	10.	189	19.775	-7.181	0.50
	ATOM 12.60	529 A	ND1BHĮS N	A	71	10.	926	19.709	-6.050	0.50
	ATOM 5.89	530 A	ND1AHIS N	A	71	10.	236	20.388	-5.942	0.50
25	ATOM 13.16	531 A	CE1BHIS C	A	71	11.	791	20.706	-6.025	0.50
	ATOM 7.95	532 A	CE1AHIS C	Α	71	11.	281	21.192	-5.898	0.50
30	ATOM 14.18	533 A	NE2BHIS	A	71	11.	618	21.438	-7.114	0.50
	ATOM 10.14	534 A	NE2AHIS N	A	71	11.9	923	21.107	-7.054	0.50

	ATOM 10.25	535 A	CD2F C	BHIS	A	71	10.617	20.883	-7.869	0.50
	ATOM 6.22	536 A	CD2 <i>I</i> C	AHIS	A	71	11.258	20.231	-7.874	0.50
5	ATOM 12.35	537 A	C C	HIS	A	71	9.806	16.875	-6.018	1.00
	ATOM 12.45	538 A	0	HIS	A	71	10.935	16.698	-5.538	1.00
10	ATOM 12.33	539 A	N N	VAL	A	72	8.697	16.657	-5.331	1.00
	ATOM 12.62	540 A	CA C	VAL	A	72	8.704	16.204	-3.960	1.00
	ATOM 12.75	541 A	CB C	VAL	A	72	7.279	16.056	-3.469	1.00
15	ATOM 12.50	542 A	CG1 C	VAL	A	72	7.248	15.256	-2.202	1.00
	ATOM 12.97	543 A	CG2 C	VAL	A	72	6.647	17.430	-3.262	1.00
20	ATOM 13.01	544 A	C C	VAL	Α	72	9.431	14.864	-3.799	1.00
	ATOM 12.02	545 A	0 0	VAL	A	72	10.333	14.707	-2.947	1.00
	ATOM 12.23		N N.		A	73	9.054	13.888	-4.615	1.00
25	ATOM 12.29	547 A	CA C	ALA	A	73	9.664	12.572	-4.521	1.00
	ATOM 12.32	548 A	CB C	ALA	Α	73	8.986	11.617	-5.440	1.00
30	ATOM 11.78	549 A	C C	ALA	Α	73	11.180	12.682	-4.850	1.00
	ATOM 11.60	550 A	0 0	ALA	A	73	11.985	11.992	-4.280	1.00

	ATOM 12.04	551 A	N N	GLY A	74	11.553	13.583	-5.742	1.00
	ATOM 11.92	552 A	CA C	GLY A	74	12.961	13.760	-6.069	1.00
5	ATOM 12.13	553 A	C C	GLY A	74	13.768	14.190	-4.845	1.00
	ATOM 11.64	554 A	0	GLY A	74	14.936	13.816	-4.693	1.00
10	ATOM 12.08	555 A	N N	SER A	75	13.157	15.015	-3.994	1.00
•	ATOM 12.08	556 A	CA C	SER A	75	13.844	15.546	-2.827	1.00
	ATOM 11.53	557 A	CB C	SER A	75	13.095	16.748	-2.267	1.00
15	ATOM 13.29	558 A	OG O	SER A	75	13.254	17.915	-3.077	1.00
	ATOM 12.05	559 A	C C	SER A	75	14.033	14.477	-1.739	1.00
20	ATOM 12.73	560 A	0	SER A	75	14.984	14.540	-0.927	1.00
•	ATOM 11.61	561 A	N N	VAL A	76	13.112	13.524	-1.676	1.00
	ATOM 11.87		CA C	VAL A	76	13.272	12.407	-0.748	1.00
25	ATOM 12.06	563 ·		VAL A	76	12.023	11.519	-0.691	1.00
	ATOM 12.75	564 A		VAL A	76	12.224	10.396	0.324	1.00
30	ATOM 11.56	565 A		VAL A	76	10.799	12.319	-0.316	1.00
	ATOM 12.11	566 A		VAL A	76	14.415	11.501	-1.173	1.00

	ATOM 10.37	567 A	0	VAL Z	A 76	15	5.280	11.158	-0.372	1.00
	ATOM 12.79	568 A	N N	LEU Z	A 77	14	4.410	11.085	-2.437	1.00
5	ATOM 12.61	569 A	CA C	LEU A	A 77	15	5.234	9.934	-2.809	1.00
	ATOM 13.05	570 A	CB C	LEU A	A 77	14	1.532	8.627	-2.425	1.00
10	ATOM 11.85	571 A	CG C	LEU A	A 77	, 13	3.050	8.419	-2.774	1.00
	ATOM 12.80	572 A	CD1 C	LEU A	77	12	2.868	8.361	-4.281	1.00
	ATOM 14.07	573 A	CD2 C	LEU A	A 77	12	2.512	7.140	-2.114	1.00
15	ATOM 13.21	574 A	C C	LEU A	A 77	15	5.676	9.847	-4.267	1.00
	ATOM 13.59	575 A	0 0	LEU A	A 77 <sub>.</sub>	16	5.181	8.810	-4.656	1.00
20	ATOM 13.72	576 - <b>A</b>	N N	GLY A	<b>A</b> 78	15	5.586	10.935	-5.022	1.00
	ATOM 14.19	577 Â	CA C	GLY A	A 78	16	5.045	10.945	-6.415	1.00
	ATOM 14.88		C C	GLY A	A 78	17	7.486	10.505	-6.506	1.00
25	ATOM 14.70	579 A	0	GLY A	A 78	18	3.322	10.998	-5.718	1.00
	ATOM 15.24	580 A	N N	ASN A	A 79	17	7.800	9.587	-7.420	1.00
30	ATOM 16.71	581 A	CA C	ASN A	79	19	).172	9.066	-7.520	1.00
	ATOM 16.08	582 · A	CB C	ASN A	79	19	204	7.542	-7.263	1.00

	ATOM 16.70	583 A	CG C	ASN	A	79	20.615	7.023	-6.904	1.00
	ATOM 15.21	584 A	OD1 O	ASN	A	79	21.438	7.754	-6.372	1.00
5	ATOM 15.92	585 A	ND2 N	ASN	A	79	20.881	5.749	-7.181	1.00
	ATOM 18.12	586 A	C C	ASN	A	79	19.877	9.353	-8.852	1.00
10	ATOM 18.96	587 A	0	ASN	A	79	20.735	8.576	-9.267	1.00
	ATOM 18.68	588 A	N N	ALA	A	80	19.559	10.458	-9.513	1.00
	ATOM 19.08	589 A	CA C	ALA	Α	80	20.316	10.838	-10.723	1.00
15	ATOM 19.15	590 A	CB C	ALA	A	80	19.381	11.169	-11.876	1.00
	ATOM 18.85	591 A	C C	ALA	A	80	21.261	11.995	-10.376	1.00
20	ATOM 18.76	592 A	0 0	ALA	A	80	22.245	11.795	-9.663	1.00
	ATOM 18.39	593 A	N.	THR	A	81	20.973	13.194	-10.841	1.00
	ATOM 18.18	594 A	CA C	THR	A	81	21.647	14.370	-10.305	1.00
25	ATOM 18.72	595 A		THR	A	81	22.229	15.222	-11.444	1.00
	ATOM 17.48	596 A	OG1 O	THR	A	81	21.202	15.535	-12.379	1.00
30	ATOM 21.52	597 A	CG2 C	THR	A		23.229	14.420	-12.289	1.00
	ATOM 17.64	598 A	C C	THR	A	81	20.650	15.185	-9.470	1.00

	ATOM 17.77	599 A	0	THR	A	81	19.466	14.858	-9.423	1.00
	ATOM 16.86	600 A	N N	ASN	A	82	21.115	16.238	-8.803	1.00
5	ATOM 16.82	601 A	CA C	ASN	A	82	20.271	16.947	-7.842	1.00
	ATOM 16.90	602 A	CB C	ASN	Α	82	19.279	17.840	-8.574	1.00
10	ATOM 18.05	603 A	CG C	ASN	A	82	19.962	18.782	-9.552	1.00
	ATOM 20.14	604 A	OD1 O	ASN	A	82	19.861	18.632	-10.804	1.00
	ATOM 12.31	605 A	ND2 N	ASN	A	82	20.650	19.760	-9.005	1.00
15	ATOM 16.16	606 A	C C	ASN	Α	82	19.541	15.941	-6.930	1.00
	ATOM . 16.88	607 A	0	ASN	A	82	18.325	15.985	-6.772	1.00
20	ATOM 15.41	608 A	N N	LYS	A	83	20.310	15.022	-6.366	1.00
	ATOM 15.60	609 A	CA C	LYS	A	83	19.767	13.853	-5.710	1.00
	ATOM 15.95		CB C	LYS	A	83	20.907	12.919	-5.287	1.00
25	ATOM 16.19	611 A		LYS	A	83	21.665	12.168	-6.415	1.00
	ATOM 19.24	612 A	CD C	LYS	Α	83	22.815	11.339	-5.811	1.00
30	ATOM 21.12	613 A		LYS	A	83	23.806	10.791	-6.833	1.00
	ATOM 20.88	. 614 A	NZ N		A	83	23.076	9.941	-7.791	1.00

	ATOM 14.74	615 A	C C		A <sub>.</sub>	83	18.966	14.243	-4.453	1.00
	ATOM 13.71	616 A	0	LYS	A	83	19.243	15.248	-3.801	1.00
5	ATOM 14.66	617 A	N N		Α	84	18.000	13.402	-4.117	1.00
	ATOM 14.40	618 A	CA C	GLY	A	84	17.337	13.439	-2.833	1.00
10	ATOM 14.38	619 A	C C	GLY	A	84	18.240	13.078	-1.664	1.00
	ATOM 14.68	620 A	0	GLY	A	84	19.372	12.683	-1.853	1.00
	ATOM 13.41	621 A	N N	MET	A	85	17.734	13.231	-0.439	1.00
15	ATOM 13.39	622 A	CA C	MET	A	85	18.586	13.079	0.753	1.00
	ATOM 13.62	623 A	CB C	MET	A	85	17.865	13.660	1.970	1.00
20	ATOM 14.10	624 A	CG C	MET	Α	85	17.446	15.132	1.799	1.00
	ATOM . 15.77	625 A	SD S	MET	Α	85	18.823	16.235	1.480	1.00
	ATOM 16.54	626 A	CE C	MET	A	85	18.801	16.373	-0.341	1.00
25	ATOM 13.55	627 · A	C C	MET	A	85	18.946	11.600	1.022	1.00
	ATOM 13.91	628 A	0 0	MET	A	85	19.975	11.302	1.623	1.00
30	ATOM 13.51	629 · A	N N	ALA	A	86	18.078	10.685	0.586	1.00
	ATOM 13.69	630 A	CA C	ALA	Α	86	18.290	9.250	0.774	.1.00

	ATOM 13.63	631 A	CB C	ALA	Α	86	17.223	8.682	1.717	1.00
	ATOM 13.59	632 A	C C	ALA	A	86	18.200	8.571	-0.589	1.00
5	ATOM 14.50	633 A	0	ALA	A	86	17.258	7.821	-0.868	1.00
	ATOM 14.33	634 A	N N	PRO	A	87	19.175	8.818	-1.445	1.00
10	ATOM 14.18	635 A	CA C	PRO	A	87	19.068	8.409	-2.859	1.00
	ATOM 14.93	636 A	CB C	PRO	A	87	20.236	9.152	-3.515	1.00
	ATOM 14.56	637 A	CG C	PRO	A	87	21.263	9.267	-2.393	1.00
15	ATOM 13.97	638 A	CD C	PRO	A	87	20.446	9.524	-1.148	1.00
	ATOM 14.68	639 <sub>.</sub> A	C C	PRO	A	87	19.146	6.901	-3.123	1.00
20	ATOM 15.65	640 A	0 0	PRO	A	87	18.943	6.474	-4.260	1.00
	ATOM 15.11	641 A	N N	GLN	A	88	19.424	6.099	-2.109	1.00
	ATOM 16.35	642 A	CA C	GLN	A	88	19.436	4.639	-2.266	1.00
25	ATOM 16.73	643 A	CB C	GLN	A	88	20.748	4.050	-1.733	1.00
	ATOM 19.50	644 A	CG C	GLN	A	88	21.900	4.262	-2.703	1.00
30	ATOM 21.39	645 A	CD C	GLN	A	88	23.267	3.916	-2.161	1.00
	ATOM 22.79	646 A	OE1 O	GLN	A	88	23.427	2.933	-1.439	1.00

	ATOM 22.41	647 A	NE2 N	GLN	A	88	24.272	4.709	-2.547	1.00
	ATOM 16.49	648 A	C C	GLN	A	88	18.228	3.976	-1.621	1.00
5	ATOM 16.50	649 A	0	GLN	A	88	18.080	2.754	-1.644	1.00
	ATOM 16.72	650 A	N N	ALA	A	89	17.347	4.786	-1.044	1.00
10	ATOM 16.78	651 A	CA C	ALA	A	89	16.056	4.279	-0.599	1.00
	ATOM 17.28	652 A	CB C	ALA	A	89	15.380	5.277	0.375	1.00
	ATOM 16.32	653 A	C C	ALA	A	89	15.139	3.996	-1.792	1.00
15	ATOM 16.81	654 A	0 0	ALA	A	89	15.212	4.648	-2.826	1.00
	ATOM 15.45	655 A	N N	ASN	A	90	14.248	3.037	-1.634	1.00
20	ATOM 15.40	656 A	CA C	ASN	A	90	13.264	2.756	-2.658	1.00
	ATOM 16.05	657 A	CB C	ASN	A	90	13.036	1.247	-2.756	1.00
	ATOM 19.92	658 A	CG C	ASN	A	90	14.076	0.549	-3.658	1.00
25	ATOM 25.00	659 A	OD1 O	ASN	A	90	15.039	1.155	-4.106	1.00
	ATOM 28.28	660 A	ND2 N	ASN	A	90	13.892	-0.736	-3.873	1.00
30	ATOM 14.01	661 A	C C	ASN	A.	90	11.942	3.486	-2.367	1.00
-	ATOM 12.81	662 A	0 0	ASN	A	90	11.668	3.834	-1.234	1.00

	ATOM 13.02	663 A	N N	LEU .	A 91	11.150	3.705	-3.410	1.00
	ATOM 13.78	664 A	CA C	LEU A	A 91	9.964	4.542	-3.381	1.00
5	ATOM 13.95	665 A	CB C	LEU A	A 91	10.022	5.524	-4.540	1.00
	ATOM 12.85	666 A	CG C	LEU A	A 91	8.861	6.472	-4.765	1.00
10	ATOM 15.80	667 A	CD1 C	LEU A	A 91	8.669	7.375	-3.571	1.00
	ATOM 13.13	668 A	CD2 C	LEU A	A 91	9.077	7.287	-6.026	1.00
	ATOM 14.15	669 A	C C	LEU A	A 91	8.661	3.762	-3.524	1.00
15	ATOM 15.63	670 A	0 0	LEU A	A 91	8.503	2.953	-4.437	1.00
	ATOM 13.69	671 A	N N	VAL A	A 92	7.716	4.055	-2.649	1.00
20	ATOM 14.00	672 A	CA C	VAL A	A 92	6.327	3.692	-2.872	1.00
	ATOM 13.15	673 A	CB C	VAL A	A 92	5.737	3.031	-1.662	1.00
	ATOM 15.32	674 A	CG1 C	VAL A	A 92	4.197	3.018	-1.767	1.00
25	ATOM 13.02	675 A	CG2 C	VAL A	A 92	6.260	1.621	-1.546	1.00
	ATOM 13.45	676 A	C C	VAL A	A 92	5.615	5.001	-3.175	1.00
30	ATOM 13.53	677 A	0 0	VAL <sub>.</sub> A	A 92	5.687	5.942	-2.376	1.00
	ATOM 13.19		N N	PHE A	A 93	4.984	5.107	-4.346	1.00

	ATOM 13.05	679 A	CA C	PHE	A	93	4.293	6.351	-4.714	1.00
	ATOM 13.57	680 A	CB C	PHE	A	93	4.899	6.964	-5.985	1.00
5	ATOM 13.50	681 A	CG C	PHE	A	93	4.484	8.388	-6.206	1.00
	ATOM 13.00	682 A	CD1 C	PHE	A	93	5.331	9.439	-5.861	1.00
10	ATOM 12.71	683 A	CE1 C	PHE	A	93	4.941	10.748	-6.023	1.00
	ATOM 11.77	684 A	CZ C	PHE	A	93	3.680	11.030	-6.515	1.00
	ATOM 12.22	685 A	CE2 C	PHE	A	93	2.832	9.998	-6.881	1.00
15	ATOM 12.44	686 A	CD2 C	PHE	A	93	3.226	8.679	-6.710	1.00
	ATOM 13.51	687 A	C C	PHE	Α	93	2.793	6.150	-4.872	1.00
20	ATOM 13.61	688 A	0 0	PHE	A	93	2.350	5.285	-5.632	1.00
	ATOM 13.35	689 A	N N	GLN	A	94	2.021	6.949	-4.150	1.00
	ATOM 13.55	690 A	CA C	GLN	A	94	0.567	6.903	-4.197	1.00
25	ATOM 12.95	691 A	CB C	GLN	A	94	-0.034	6.775	-2.786	1.00
	ATOM 13.25	692 A	CG C	GLN	Α	94	0.383	5.493	-2.078	1.00
30	ATOM 14.07	693 A	CD C	GLN	A	94	0.065	5.494	-0.589	1.00
	ATOM 16.83	694 A	OE1 O	GLN	A	94	0.598	6.311	0.157	1.00

	ATOM 13.83	695 A	NE2 N	GLN	A	94	-0.813	4.578	-0.158	1.00
	ATOM 13.81	696 A	C C	GLN	A	94	0.118	8.195	-4.841	1.00
5	ATOM 12.11	697 <b>A</b>	0 0	GLN	A	94	0.197	9.289	-4.236	1.00
	ATOM 14.33	698 A	N N	SER	A	95	-0.266	8.072	-6.110	1.00
10	ATOM 14.08	699 A	CA C	SER	A	95	-0.793	9.190	-6.893	1.00
	ATOM 13.95	700 A	CB C	SER	A	95	-0.743	8.850	-8.380	1.00
	ATOM 11.92	701 A	OG O	SER	A	95	-1.337	9.864	-9.152	1.00
15	ATOM 14.82	702 A	C C	SER	A	95	-2.221	9.519	-6.494	1.00
	ATOM 14.73	703 A	0 0	SER	A .	95	-3.150	8.743	-6.780	1.00
20	ATOM 15.21	704 A	N N	ILE	A	96	-2.404	10.681	-5.852	1.00
	ATOM 15.55	705 A	CA C	ILE	A	96	-3.699	11.049	-5.277	1.00
	ATOM 15.92	706 A	CB C	ILE	A	96	-3.560	11.482	-3.782	1.00
25	ATOM 16.08	707 A	CG1 C	ILE	A	96	-2.466	12.548	-3.597	1.00
	ATOM 17.02	708 A	CD1 C	ILE	A	96	-2.367	13.122	-2.196	1.00
30	ATOM 16.70	709 A	CG2 C	ILE	A	96	-3.257	10.273	-2.915	1.00
	ATOM 15.93	710 A		ILE	A	96	-4.398	12.158	-6.043	1.00

			_			0.5	E 47E	10 500	F (()	1.00
	ATOM 14.84	711 A	0	ILE	A	96	-5.475	12.590	-5.660	
	ATOM 16.32	712 A	N N	MET	A	97	-3.797	12.640	-7.119	1.00
5	ATOM 18.17	713 A	CA C	MET	A	97	-4.440	13.700	-7.889	1.00
	ATOM 18.20	714 A	CB C	MET	A	97	-3.471	14.346	-8.884	1.00
10	ATOM 21.58	715 A	CG C	MET	A	97	-4.107	15.480	-9.688	1.00
	ATOM 25.41	716 A	SD S	MET	Α	97	-2.949	16.297	-10.814	1.00
	ATOM 31.75	717 A	CE C	MET	A	97	-3.900	16.196	-12.225	1.00
15	ATOM 18.32	718 A	C C	MET	Α	97	-5.647	13.114	-8.641	1.00
	ATOM 18.26	719 A	0	MET	A	97	-5.537	12.054	-9.249	1.00
20	ATOM 19.35	720 A	N N	ASP	A	98	6.780	13.807	-8.568	1.00
	ATOM 20.45	721 A	CA C	ASP	A	98	-8.020	13.369	-9.217	1.00
	ATOM 20.39	722 A	CB C	ASP	A	98	-9.268	13.714	-8.375	1.00
25	ATOM 21.41	723 A	CG C	ASP	A	98	-9.367	15.170	-8.021	1.00
	ATOM 22.52	724 A	OD1 O	ASP	A	98	-9.234	16.024	-8.928	1.00
30	ATOM 20.32	725 A	OD2 O	ASP	A	98	-9.599	15.575	-6.847	1.00
	ATOM 20.49	726 A	C C	ASP	A	98	-8.093	14.004	-10.592	1.00

	ATOM 19.61	727 A	0	ASP	A	98	-7.168	14.690	-10.996	1.00
	ATOM 21.70	728 A	N N	SER	A	99	-9.170	13.747	-11.321	1.00
5	ATOM 23.74	729 A	CA C	SER	A	99	-9.252	14.202	-12.703	1.00
	ATOM 24.07	730 A	CB C	SER	A	99	-10.202	13.301	-13.510	1.00
10	ATOM 25.19	731 A	OG O	SER	A	99	-11.497	13.436	-12.986	1.00
	ATOM 24.80	732 A	C C	SER	A	99	-9.727	15.660	-12.749	1.00
	ATOM 27.46	733 A	0	SER	A	99	-9.696	16.286	-13.812	1.00
15	ATOM 24.38	734 A	N N	GLY	A	100	-10.152	16.203	-11.611	1.00
	ATOM 25.17	735 A	CA C	GLY	A	100	-10.425	17.621	-11.488	1.00
20	ATOM 25.36	736 A	C C	GLY	A	100	-9.262	18.470	-10.968	1.00
	ATOM 26.29	737 A	0	GLY	A	100	-9.475	19.606	-10.557	1.00
	ATOM 25.13	738 A	N N	GLY	Α	101	-8.047	17.933	-10.964	1.00
25	ATOM 24.90	739 A	CA <u>C</u>	GLY	Α	101	-6.873	18.715	-10.573	1.00
	ATOM 24.55	740 A	C C	GLY	A	101	-6.541	18.760	-9.076	1.00
30	ATOM 26.15	741 A	0	GLY	A	101	-5.425	19.133	-8.713	1.00
	ATOM 22.32	742 A	N N	GLY	A	102	-7.490	18.406	-8.221	1.00

	ATOM 21.84	743 A	CA C	GLY	A	102	-7.258	18.339	-6.783	1.00
	ATOM 20.73	744 A	C C	GLY	Α	102	-6.703	17.008	-6.267	1.00
5	ATOM 19.11	745 A	0	GLY	A	102	-6.172	16.204	-7.021	1.00
	ATOM 19.97	746 A	N N	LEU	A	103	-6.814	16.794	-4.959	1.00
10	ATOM 19.19	747 A	CA C	LEU	A	103	-6.225	15.634	-4.294	1.00
	ATOM 18.87	748 A	CB C	LEU	Α	103	-5.346	16.094	-3.131	1.00
	ATOM 18.31	749 A	CG C	LEU	Α	103	-4.169	16.986	-3.552	1.00
15	ATOM 17.54	750 A	CD1 C	LEU	Α	103	-3.298	17.397	-2.354	1.00
	ATOM 19.64	751 A	CD2 C	LEU	A	103	-3.341	16.297	-4.607	1.00
20	ATOM 19.31	752 A	C C	LEU	A	103	-7.307	14.676	-3.809	1.00
	ATOM 18.44	753 A	0	LEU	A	103	-7.179	14.018	-2.750	1.00
	ATOM 18.93	754 A	N N	GLY	A	104	-8.371	14.586	-4.604	1.00
25	ATOM 18.78	755 A	ĆA C	GLY	A	104	-9.537	13.780	-4.260	1.00
	ATOM 18.26	756 A	C C	GLY	A	104	-9.259	12.298	-4.234	1.00
30	ATOM 19.17	757 A	0	GLY	Α	104	-10.078	11.506	-3.780	1.00
	ATOM 17.54	758 A	N N	GLY	A	105	-8.094	11.886	-4.703	1.00

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,	ATOM 17.23	759 A	CA C	GLY	Α	105	-7.698	10.500	-4.520	1.00
	ATOM 16.85	760 A	C C	GLY	A	105	-7.395	10.091	-3.075	1.00
5	ATOM 15.88	761 A	0	GLY	A	105	-7.319	8.895	-2.731	1.00
	ATOM 16.62	762 A	N N	LEU	Α	106	-7.263	11.067	-2.194	1.00
10	ATOM 16.79	763 A	CA C	LEU	A	106	-7.137	10.729	-0.777	1.00
	ATOM 16.05	764 A	CB C	LEU	A	106	-6.892	11.975	0.048	1.00
	ATOM 14.68	765 A	CG C	LEU	A	106	-5.519	12.560	-0.204	1.00
15	ATOM 16.20	766 A	CD1 C	LEU	A	106	-5.479	13.986	0.274	1.00
	ATOM 13.15	767 A	CD2 C	LEU	A	106	-4.425	11.707	0.507	1.00
20	ATOM 17.90	768 A	C C	LEU	A	106	-8.423	10.056	-0.304	1.00
	ATOM 18.63	769 A	0	LEU	A.	106	-9.513	10.553	-0.587	1.00
	ATOM 18.42	770 A	N N	PRO	Α	107	-8.318	8.932	0.387	1.00
25	ATOM 19.35	771 A	CA C	PRO	A	107	-9.506	8.280	0.977	1.00
	ATOM 19.15	772 A	CB C	PRO	A	107	-8.963	6.932	1.430	1.00
30	ATOM 19.19	773 A	CG C	PRO-	A	107	-7.537	7.286	1.774	1.00
	ATOM 18.63	774 A	CD C	PRO	Α	107	-7.089	8.162	0.640	1.00

	ATOM 18.88	775 A	C C	PRO	Α	107	-10.070	9.036	2.178	1.00
	ATOM 19.33	776 A	0 0	PRO	Α	107	-9.340	9.724	2.886	1.00
5 ·	ATOM 19.46	777 A	N N	ALA	Α	108	-11.367	8.910	2.408	1.00
	ATOM 19.50	778 A	CA C	ALA	Α	108	-12.022	9.562	3.530	1.00
10	ATOM 20.76	779 A	CB C	ALA	Α	108	-13.514	9.168	3.585	1.00
	ATOM 18.72	780 A	C C	ALA	A	108	-11.359	9.229	4.875	1.00
	ATOM 19.17	781 A	0	ALA	Α	108	-11.229	10.093	5.727	1.00
15	ATOM 18.94	782 A	N N	ASN	Α	109	-11.007	7.964	5.069	1.00
	ATOM 19.10	783 A	CA C	ASN	Α	109	-10.193	7.535	6.209	1.00
20	ATOM 19.41	784 A	CB C	ASN	Α	109	-10.691	6.206	6.773	1.00
	ATOM 22.66	785 A	CG C	ASN	Α	109	-9.990	5.834	8.073	1.00
,	ATOM 19.31	786 A	OD1 O	ASN	A	109	-8.872	6.295	8.349	1.00
25	ATOM 25.73	787 A	ND2 N	ASN	Α	109	-10.665	5.018	8.908	1.00
	ATOM 17.97	788 A	C C	ASN	Α	109	-8.731	7.392	5.804	1.00
30	ATOM 17.31	789 A		ASN	Α	109	-8.353	6.446	5.088	1.00
	ATOM 16.66	790 A		LEU	A <sub>,</sub>	110	-7.895	8.325	6.245	1.00

	ATOM 15.50	791 A	CA C	LEU	A	110	-6.48	9 8.277	5.862	1.00
	ATOM 15.65	792 A	CB C	LEU	A	110	-5.73	8 9.502	6.406	1.00
5	ATOM 13.74	793 A	CG C	LEU	A	110	-6.09	6 10.831	5.749	1.00
	ATOM 16.06	794 A	CD1 C	LEU	A	110	-5.29	4 11.932	6.373	1.00
10	ATOM 13.53	795 A	CD2 C	LEU	A	110	-5.87	3 10.768	4.256	1.00
	ATOM 15.96	796 A	C C	LEU	A	110	-5.78	4 ,7.006	6.285	1.00
	ATOM 16.04	79 <b>7</b> A	0	LEU	Α	110	-4.75	6.660	5.719	1.00
15	ATOM 16.18	798 A	N N	GLN	Α	111	-6.29	6.283	7.276	1.00
	ATOM 16.61	799 A	CA C	GLN	A	111	-5.63	5 5.034	7.655	1.00
20	ATOM 17.82	800 A	CB C	GLN	Α	111	-6.31	7 4.377	8.871	1.00
	ATOM 17.25	801 A	CG C	GLN	A	111	-6.33	5.320	10.077	1.00
	ATOM 20.40	802 A	CD C	GLN	Α	111	-6.58	4.625	11.399	1.00
25	ATOM 21.99	803 A	OE1 O	GLN	Α	111	-5.93	4 3.635	11.699	1.00
	ATOM 19.23	804 A	NE2 N	GLN	Α	111	-7.51	.3 5.163	12.202	1.00
30	ATOM 17.45	805 A	C C	GLN	Α	111	-5.56		6.461	1.00
	ATOM 17.74	806 A	0 0	GLN	A	111	-4.60	3.323	6.312	1.00

	ATOM 16.47	807 A	N N	THR	A	112	-6.522	4.195	5.548	1.00
	ATOM 16.12	808 A	CA C	THR	A	112	-6.483	3.418	4.309	1.00
5	ATOM 16.21	809 A	CB C	THR	Α	112	-7.756	3.733	3.510	1.00
	ATOM 17.07	810 A	OG1 O	THR	A	112	-8.900	3.480	4.333	1.00
10	ATOM 16.70	811 A	CG2 C	THR	A	112	-7.909	2.838	2.305	1.00
	ATOM 15.86	812 A	C C	THR	A	112	-5.252	3.711	3.442	1.00
	ATOM 15.50	813 A	0 0	THR	A	112	-4.623	2.789	2.869	1.00
15	ATOM 14.75	814 A	N N	LEU	A	113	-4.933	4.995	3.303	1.00
	ATOM 14.05	815 A	CA C	LEU	A	113	-3.742	5.413	2.558	1.00
20	ATOM 14.27	816 A	CB C	LEU	A	113	-3.677	6.941	2.557	1.00
	ATOM 14.53	817 A	CG C	LEU	A	113	-2.549	7.597	1.807	1.00
	ATOM 16.65	818 A	CD1 C	LEU	A	113	-2.840	7.473	0.297	1.00
25	ATOM 13.95	819 A	CD2 C	LEU	A	113	-2.412	9.039	2.212	1.00
	ATOM 13.77	820 A	C C	LEU	A	113	-2.478	4.836	3.212	1.00
30	ATOM 13.55	821 A	0	LEU	Α	113	-1.625	4.238	2.550	1.00
	ATOM 12.95	822 A	N N	PHE	Α	114	-2.361	5.016	4.523	1.00

	ATOM	823		Α	114	-1.182	4.528	5.223	1.00
	13.04	A	C				5 040	C C 4 F	1.00
	ATOM 12.56	824 A	CB PHE C	Α	114	-1.154	5.049	6.645	1.00
5	ATOM 11.79	825 A	CG PHE C	A	114	-1.331	6.551	6.743	1.00
	ATOM 12.07	826 A	CD1 PHE C	A	114	-0.639	7.402	5.902	1.00
10	ATOM 12.47	827 A	CE1 PHE C	A	114	-0.785	8.781	5.986	1.00
	ATOM 13.57	828 A	CZ PHE C	A	114	-1.662	9.323	6.921	1.00
	ATOM 11.94	829 A	CE2 PHE	A	114	-2.365	8.470	7.754	1.00
15	ATOM 9.85	830 A	CD2 PHE C	A	114	-2.186	7.100	7.663	1.00
	ATOM 13.86	831 A	C PHE C	A	114	-1.060	3.003	5.171	1.00
20	ATOM 12.73	832 A	O PHE O	Α	114	0.063	2.461	5.004	1.00
	ATOM 14.04	833 A	N SER N	A	115	-2.196	2.306	5.277	1.00
	ATOM 14.17		CA SER C	Α	115	-2.148	0.848	5.292	1.00
25		835 A		Α	115	-3.527	0.252	5.640	0.50
	ATOM 14.55	836 A	CB ASER C	Α	115	-3.457	0.215	5.769	0.50
30	ATOM 10.51	837 A	OG BSER O	Α	115	-3.970	0.566	6.958	0.50
`	ATOM 18.03	838 A	OG ASER O	A	115	-4.544	0.608	4.978	0.50

ATOM 14.11	839 A	C C	SER	Α	115	-1.677	0.296	3.943	1.00
ATOM 13.43	840 A	0	SER	Α	115	-0.932	-0.663	3.909	1.00
ATOM 14.73	841 A	N N	GLN	A	116	-2.108	0.890	2.832	1.00
ATOM 14.53	842 A	CA C	GLN	A	116	-1.656	0.442	1.513	1.00
ATOM . 15.81	843 A	CB C	GLN	Α	116	-2.394	1.234	0.417	1.00
ATOM 15.88	844 A	CG C	GLN	Α	116	-1.947	0.951	-1.038	1.00
ATOM 16.75	845. A	CD . C	GLN	Α	116	-2.601	1.886	-2.007	1.00
ATOM 14.56	846 A	OE1 O	GLN	Α	116	-2.629	3.086	-1.747	1.00
ATOM 14.07	847 A	NE2 N	GLN	A	116	-3.200	1.346	-3.106	1.00
ATOM	848 A	C C	GLN	Α	116	-0.131	0.571	1.375	1.00
ATOM	849	0	GLN	A	116	0.554	-0.336	0.861	1.00
ATOM	850	N	ALA	A	117	0.407	1.679	1.862	1.00
ATOM	851	CA	ALĄ	Α	117	1.838		1.795	1.00
ATOM	852	СВ	ALA	Α	117	2.152		2.151	1.00
ATOM	853	С	ALĄ	А	117	2.608	0.972	2.714	1.00
ATOM	854	0	ALA	Α	117	3.666	0.472	2.344	1.00
	14.11 ATOM 13.43 ATOM 14.73 ATOM 14.53 ATOM 15.81 ATOM 15.88 ATOM 16.75 ATOM 14.56 ATOM 14.07 ATOM 14.07 ATOM 14.37 ATOM 13.34 ATOM 13.34 ATOM 13.34 ATOM 13.79 ATOM 13.79 ATOM 13.79	ATOM 841 14.11 A ATOM 840 13.43 A ATOM 841 14.73 A ATOM 842 14.53 A ATOM 843 15.81 A ATOM 845 16.75 A ATOM 846 14.56 A ATOM 847 14.07 A ATOM 847 14.07 A ATOM 848 14.16 A ATOM 849 14.37 A ATOM 850 13.34 A ATOM 851 13.79 A ATOM 851 13.79 A ATOM 853 13.17 A ATOM 853 13.17 A	ATOM	ATOM	ATOM	ATOM	14.11 A C  ATOM 840 O SER A 115 -0.932 13.43 A O SER A 116 -2.108  ATOM 841 N GLN A 116 -2.108  ATOM 842 CA GLN A 116 -1.656 14.53 A C  ATOM 843 CB GLN A 116 -2.394 15.81 A C  ATOM 845 CD GLN A 116 -1.947 15.88 A C  ATOM 846 OE1 GLN A 116 -2.601 14.56 A O  ATOM 847 NE2 GLN A 116 -2.629 14.07 A N  ATOM 848 C GLN A 116 -3.200 ATOM 849 O GLN A 116 -0.131 14.16 A C  ATOM 850 N ALA A 117 0.407 13.34 A N  ATOM 851 CA ALA A 117 1.838 13.79 A C  ATOM 852 CB ALA A 117 2.608 13.17 A C  ATOM 853 C ALA A 117 2.608 13.17 A C	14.11 A C  ATOM 840 O SER A 115 -0.932 -0.663 13.43 A O  ATOM 841 N GLN A 116 -2.108 0.890 14.73 A N  ATOM 842 CA GLN A 116 -1.656 0.442 14.53 A C  ATOM 843 CB GLN A 116 -2.394 1.234 15.81 A C  ATOM 844 CG GLN A 116 -1.947 0.951 15.88 A C  ATOM 845 CD GLN A 116 -2.601 1.886 16.75 A C  ATOM 846 OE1 GLN A 116 -2.601 1.886 14.56 A O  ATOM 847 NE2 GLN A 116 -3.200 1.346 14.07 A N  ATOM 848 C GLN A 116 -0.131 0.571 14.16 A C  ATOM 849 O GLN A 116 -0.131 0.571 14.16 A C  ATOM 850 N ALA A 117 0.407 1.679 13.34 A N  ATOM 851 CA ALA A 117 1.838 1.930 13.79 A C  ATOM 852 CB ALA A 117 2.152 3.408 13.17 A C  ATOM 853 C ALA A 117 2.608 0.972 13.17 A C  ATOM 854 O ALA A 117 3.666 0.472	ATOM 844 CG GLN A 116 -2.601 1.886 -2.007 16.75 A C  ATOM 845 CD GLN A 116 -2.601 1.886 -2.007 16.75 A C  ATOM 847 NE2 GLN A 116 -3.200 1.346 -3.106 14.07 A N  ATOM 848 C GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 O GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 C GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 847 NE2 GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 O GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 C GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 C GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 C GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 849 C GLN A 116 -0.131 0.571 1.375 14.16 A C  ATOM 850 N ALA A 117 0.407 1.679 1.862 13.34 A N  ATOM 851 CA ALA A 117 1.838 1.930 1.795 13.79 A C  ATOM 852 CB ALA A 117 2.152 3.408 2.151 13.52 A C  ATOM 853 C ALA A 117 2.608 0.972 2.714 13.17 A C  ATOM 854 O ALA A 117 3.666 0.472 2.344

	ATOM 13.32	855 A	N N	TYR	A	118	2.071	0.740	3.908	1.00
	ATOM 13.82	856 A	CA C	TYR	Α	118	2.679	-0.161	4.877	1.00
5	ATOM 14.02	857 A	CB C	TYR	Α	118	1.878	-0.177	6.190	1.00
	ATOM 17.04	858 A	CG C	TYR	Α	118	2.636	-0.861	7.324	1.00
10	ATOM 20.14	859 A		TYR	Α	118	2.472	-2.216	7.589	1.00
10	ATOM 24.14	860 A	+	TYR	Α	118	3.186	-2.839	8.640	1.00
	ATOM 23.61	861 A	CZ C	TYR	A	118	4.041	-2.071	9.409	1.00
15	ATOM 28.49	862 A	ОН	TYR	A	118	4.762	-2.631	10.442	1.00
	ATOM 20.69	863 A		TYR	Α	118	4.194	-0.725	9.155	1.00
20	ATOM 18.61	864 A		TYR	A	118	3.501	-0.135	8.136	1.00
	ATOM 14.18	865	C . C	TYR	A	118	2.782	-1.576	4.294	1.00
	ATOM 14.05		0	TYR	Α	118	3.838	-2.228	4.363	1.00
25	ATOM 14.24	867 A		SER	Α	119	1.705	-2.024	3.669	1.00
	ATOM 15.13	868 A	CA C	SER	Α	119	1.684	-3.358	3.064	1.00
30	ATOM 14.77	869 A	CB C	SER	A	119	0.288	-3.660	2.544	1.00
50	ATOM 13.56	•		SER	Α	119	-0.609	-3.744	3.638	1.00

ATOM 871 C SER A 119 2.752 -3.53 15.67 A C ATOM 872 O SER A 119 3.313 -4.60 15.80 A O 5 ATOM 873 N ALA A 120 3.052 -2.46	2 1.818 1.00 1 1.254 1.00
15.80 A O	1 1.254 1.00
E ATTOM 072 N ALA A 120 2 052 2 46	
5 ATOM 873 N ALA A 120 3.052 -2.46 16.24 A N	8 0.204 1.00
ATOM 874 CA ALA A 120 4.085 -2.48 15.93 A C	
ATOM 875 CB ALA A 120 3.847 -1.35 10 16.16 A C	2 -0.759 1.00
ATOM 876 C ALA A 120 5.504 -2.40 16.13 A C	5 0.767 1.00
ATOM 877 O ALA A 120 6.474 -2.47 16.93 A O	3 0.030 1.00
15 ATOM 878 N GLY A 121 5.626 -2.24 16.23 A N	9 2.083 1.00
ATOM 879 CA GLY A 121 6.917 -2.24 15.35 A C	9 2.747 1.00
ATOM 880 C GLY A 121 7.400 -0.883	3 3.247 1.00
ATOM 881 O GLY A 121 8.466 -0.81	1 3.893 1.00
	5 2.977 1.00
25 ATOM 883 CA ALA A 122 7.110 1.523	2 3.443 1.00
ATOM 884 CB ALA A 122 6.273 2.633	2 2.831 1.00
ATOM 885 C ALA A 122 7.057 1.63	5 4.964 1.00
30 14.35 A C  ATOM 886 O ALA A 122 6.078 1.230 15.21 A O	5.574 1.00

ATOM 887 N ARG A 123 8.077 2.223 5.57 13.62 A N  ATOM 888 CA ARG A 123 8.013 2.499 7.00 12.85 A C  5 ATOM 889 CB ARG A 123 9.065 1.689 7.76 12.85 A C  ATOM 890 CG ARG A 123 8.870 0.162 7.59 13.74 A C  ATOM 891 CD ARG A 123 7.584 -0.334 8.29 10 14.35 A C  ATOM 892 NE ARG A 123 7.396 -1.786 8.18 14.77 A N  ATOM 893 CZ ARG A 123 6.676 -2.389 7.255	
12.85 A C  5 ATOM 889 CB ARG A 123 9.065 1.689 7.76 12.85 A C  ATOM 890 CG ARG A 123 8.870 0.162 7.59 13.74 A C  ATOM 891 CD ARG A 123 7.584 -0.334 8.29 10 14.35 A C  ATOM 892 NE ARG A 123 7.396 -1.786 8.189 14.77 A N	0 1.00
12.85 A C  ATOM 890 CG ARG A 123 8.870 0.162 7.59 13.74 A C  ATOM 891 CD ARG A 123 7.584 -0.334 8.29 10 14.35 A C  ATOM 892 NE ARG A 123 7.396 -1.786 8.186 14.77 A N	3 1.00
13.74 A C  ATOM 891 CD ARG A 123 7.584 -0.334 8.29  10 14.35 A C  ATOM 892 NE ARG A 123 7.396 -1.786 8.18  14.77 A N	1.00
10 14.35 A C  ATOM 892 NE ARG A 123 7.396 -1.786 8.189 14.77 A N	7 1.00
14.77 A N	1.00
ATOM 893 CZ ARG A 123 6.676 -2.389 7.25	7 1.00
16.63 A C	3 1.00
15 ATOM 894 NH1 ARG A 123 6.039 -1.678 6.33 15.68 A N	7 1.00
ATOM 895 NH2 ARG A 123 6.579 -3.719 7.24	1.00
ATOM 896 C ARG A 123 8.132 3.987 7.29 20 12.72 A C	3 1.00
ATOM 897 O ARG A 123 8.116 4.418 8.44 12.15 A O	3 1.00
ATOM 898 N ILE A 124 8.225 4.773 6.23 12.67 A N	1.00
25 ATOM 899 CA ILE A 124 8.177 6.218 6.34 12.97 A C	5 1.00
ATOM 900 CB ILE A 124 9.554 6.814 6.029	5 1.00
12.64 A C  ATOM 901 CG1 ILE A 124 10.619 6.262 6.985	5 1.00
30 13.71 A C  ATOM 902 CD1 ILE A 124 12.068 6.395 6.480 14.82 A C	1.00

	ATOM 13.97	903 A	CG2 C	ILE	A	124		9.478	8.348	6.061	1.00
	ATOM 12.91	904 A	C C	ILE	Α	124		7.160	6.695	5.324	1.00
5	ATOM 13.07	905 A	0 0	ILE	Α	124		7.132	6.195	4.210	1.00
	ATOM 12.94	906 A	N N		A	125		6.365	7.696	5.671	1.00
10	ATOM 12.77	907 A	CA C	HIS	A	125		5.252	8.100	4.823	1.00
	ATOM 13.00	908 A	CB C	HIS	Α	125		3.894	7.549	5.353	1.00
	ATOM 15.91	909 A	CG C	HIS	A	125	- (	2.806	7.650	4.334	1.00
15	ATOM 13.47	910 A	ND1 N	HIS	Α	125		2.428	8.850	3.783	1.00
	ATOM 16.40	911 A	CE1 C	HIS	Α	125		1.547	8.632	2.821	1.00
20	ATOM 16.49	912 A	NE2 N	HIS	Α	125		1.312	7.333	2.756	1.00
	ATOM 18.35	913 A	CD2 C	HIS	Α	125		2.072	6.699	3.705 .	1.00
	ATOM 12.62	914 A		HIS	A	125		5.223	9.620	4.828	1.00
25	ATOM 12.04		0 0	HIS	Α	125		5.053	10.202	5.893	1.00
	ATOM 12.71	916 A	N N	THR	A	126		5.401	10.268	3.674	1.00
30	ATOM 12.63	917 A	CA C	THR	<b>. A</b> .	126		5.527	11.738	3.641	1.00
	ATOM 12.63	918 A	CB C	THR	Α	126		6.984	12.142	3.302	1.00

	ATOM 12.18	919 A	0G1 0	THR	A	126	7.121	13.560	3.334	1.00
	ATOM 12.36	920 A	CG2 C	THR	A	126	7.395	11.747	1.864	1.00
5	ATOM 12.60	921 A	C C	THR	A	126	4.498	12.426	2.735	1.00
	ATOM 12.62	922 A	0	THR	A	126	4.166	11.931	1.652	1.00
10	ATOM 12.52	923 A	N N	ASN	A	127	4.010	13.572	3.200	1.00
	ATOM 12.84	924 A	CA C	ASN	A	127	2.778	14.189	2.696	1.00
	ATOM 13.04	925 A	CB C	ASN	A	127	1.599	13.811	3.605	1.00
15	ATOM 13.25	926 A	CG C	ASN	A	127	1.433	12.325	3.720	1.00
	ATOM 13.15	927 A	OD1 O	ASN	A	127	1.916	11.686	4.690	1.00
20	ATOM 9.82	928 A	ND2 N	ASN	Α	127	0.814	11.740	2.712	1.00
	ATOM 12.70	929 A	C C	ASN	A	127	2.894	15.706	2.637	1.00
	ATOM 13.27	930 A	0 0	ASN	A	127	2.798	16.390	3.661	1.00
25	ATOM 12.76	931 A	N N	SER	A	128	3.103	16.211	1.435	1.00
	ATOM 13.02	932 A	CA C	SER	A	128	3.277	17.640	1.162	1.00
30	ATOM 12.57	933 A	CB C	SER	A	128	4.308	17.831	0.043	1.00
	ATOM 12.52	934 A	OG O	SER	A	128	5.608	17.510	0.485	1.00

	ATOM 13.42	935 A	C C	SER	A	128		1.927	18.238	0.748	1.00
	ATOM 13.82	936 A	0 0	SER	A	128		1.763	18.767	-0.372	1.00
5	ATOM 13.86	937 A	N N	TRP	A	129		0.968	18.129	1.663	1.00
	ATOM 13.67	938 A	CA C	TRP	A	129		-0.392	18.616	1.465	1.00
10	ATOM 13.88	939 A	CB C	TRP	A	129		-1.215	17.648	0.602	1.00
	ATOM 13.08	940 A	CG C	TRP	Α	129		-1.130	16.180	0.964	1.00
	ATOM 14.80	941 A	CD1 C	TRP	A	129		-0.305	15.232	0.391	1.00
15	ATOM 12.40	942 . A	NE1 N	TRP	A	129		-0.531	13.997	0.956	1.00
	ATOM 13.40	943 A	CE2 C	TRP	Α	129		-1.518	14.122	1.900	1.00
20	ATOM 12.64	944 A	CD2 C	TRP	Α	129		-1.924	15.480	1.921	1.00
	ATOM 14.15	945 A	CE3 C	TRP	A	129		-2.948	15.857	2.806	1.00
	ATOM 13.25	946 A	CZ3	TRP	A	129		-3.504	14.910	3.614	1.00
25	ATOM 13.78	947 A	CH2 C	TRP	A	129		-3.082	13.566	3.559	1.00
	ATOM 12.56	948 A	CZ2 C	TRP	Α	129		-2.101	13.158	2.711	1.00
30	ATOM 14.44	949 A	•	TRP	Α	129		-1.089	18.859	2.782	1.00
	ATOM 14.19	950 A	0 0	TRP	A	129	-	-0.612	18.460	3.876	1.00

	ATOM 14.75	951 A	N N	GLY A	A 130	-2.224	19.538	2.694	1.00
	ATOM 15.45	952 A	CA C	GLY A	130	-3.004	19.834	3.866	1.00
5	ATOM 16.66	953 A	C C	GLY A	A 130	-4.173	20.744	3.563	1.00
	ATOM 16.04	954 A	0	GLY A	A 130	-4.203	21.394	2.518	1.00
10	ATOM 16.87	955 A	N N	ALA A	A 131	-5.139	20.754	4.478	1.00
	ATOM 18.19	956 A	CA C	ALA A	131	-6.222	21.733	4.484	1.00
	ATOM 17.33	957 A	CB C	ALA A	131	-7.515	21.097	4.983	1.00
15	ATOM 19.54	958 A	C C	ALA A	A 131	-5.843	22.852	5.423	1.00
	ATOM 20.18	959 A	0 0	ALA A	131	-5.562	22.590	6.592	1.00
20	ATOM 20.97	960 A	N N	PRO P	132	-5.869	24.090	4.942	1.00
	ATOM 21.46	961 A	CA C	PRO A	132	-5.513	25.253	5.763	1.00
	ATOM 21.95		CB C	PRO A	132	-5.260	26.346	4.724	1.00
25	ATOM 22.18	963 A		PRO A	. 132	-6.060	25.967	3.546	1.00
	ATOM 21.43	964 A	CD C	PRO A	. 132	-6.220	24.462	3.564	1.00
30		· 965 A·	C C	PRO A	132	-6.595	25.676	6.753	1.00
	ATOM 24.13	966 A	0 0	PRO A	. 132	-7.272	26.703	6.555	1.00

	ATOM 22.71	967 A	N N	VAL	A	133		-6.708	24.912	7.833	1.00
	ATOM 23.39	968 A	CA C	VAL	A	133		-7.723	25.086	8.850	1.00
5	ATOM 23.48	969 A	CB C	VAL	A	133		-8.349	23.712	9.223	1.00
	ATOM 25.68	970 A	CG1 C	VAL	A	133		-9.115	23.133	8.045	1.00
10	ATOM 24.53	971 . A	CG2 C	VAL	A	133		-7.269	22.750	9.687	1.00
	ATOM 23.23	972 A	C	VAL	A	133	-	-7.223	25.742	10.150	1.00
	ATOM 22.57	973 A	0 .	VAL	A	133		-7.855	25.599	11.185	1.00
15	ATOM 23.10	974 . A	N N	ASN	A	134		-6.094	26.437	10.098	1.00
	ATOM 23.36	975 A	CA C	ASN	A	134		-5.660	27.279	11.201	1.00
20	ATOM 24.40	976 A	CB C	ASN	A	134		-6.583	28.512	11.310	1.00
	ATOM 26.68	977 A	CG C	ASN	A	134		-6.491	29.413	10.082	1.00
	ATOM 34.40	978 A	OD1 O	ASN	Α	134		-7.489	30.000	9.650	1.00
25	ATOM 28.87	979 A	ND2 N	ASN	Α	134		-5.315	29.478	9.482	1.00
	ATOM 22.43	980 A	C C	ASN	A	134		-5.588	26.561	12.535	1.00
30	ATOM 21.30	981 A	0 0	ASN	A	134		-6.210	26.971	13.510	1.00
	ATOM 21.06	982 A	N N	GLY	Α	135		-4.844	25.458	12.574	1.00

	ATOM 20.36	983 A	CA C	GLY A	135	-4.548	24.840	13.846	1.00
	ATOM 19.66	984 A	C C	GLY A	. 135	-5.541	23.818	14.308	1.00
5	ATOM 18.95	985 A	0	GLY A	. 135	-5.320	23.200	15.327	1.00
	ATOM 19.08	986 A	N N	ALA A	136	-6.613	23.595	13.557	1.00
10	ATOM 19.00	987 A	CA C	ALA A	136	-7.609	22.643	14.006	1.00
	ATOM 19.34	988 A	CB C	ALA A	136	-8.925	22.778	13.199	1.00
	ATOM 19.31	989 A	C C	ALA A	136	-7.098	21.206	13.893	1.00
15	ATOM 18.44	990 A	0	ALA A	136	-6.354	20.851	12.952	1.00
	ATOM 18.56	991 A	N N	TYR A	137	-7.568	20.407	14.841	1.00
20	ATOM 18.99	992 A	CA C	TYR A	137	-7.341	18.979	14.907	1.00
	ATOM 18.67	993 A	CB C	TYR A	137	-7.112	18.588	16.367	1.00
	ATOM 19.68	994 A	CG C	TYR A	137	-6.637	17.175	16.588	1.00
25	ATOM 19.55	995 A	CD1 C	TYR A	137	-7.537	16.173	16.885	1.00
	ATOM 21.07	996 A	CE1 C	TYR A	137	-7.112	14.855	17.099	1.00
30	ATOM 20.92	997 A	CZ C	TYR A	137	-5.765	14.548	17.045	1.00
	ATOM 20.20	998 A	ОН	TYR A	137	-5.371	13.250	17.265	1.00

	ATOM 20.35	999 A		TYR	Α	137	-4.83	7 15.538	16.754	1.00
	ATOM 19.75	1000 A	CD2 C	TYR	A	137	-5.278	3 16.848	16.522	1.00
5	ATOM 18.91	1001 A		TYR	A	137	-8.60	0 18.314	14.337	1.00
	ATOM 18.41	1002 A	0 0	TYR	A	137	-9.64	8 18.229	14.994	1.00
10	ATOM 18.62			THR	A	138	-8.48	1 17.872	13.091	1.00
	ATOM 17.86	1004 A		THR	A	138	-9.608	3 17.401	12.329	1.00
	ATOM 18.02	1005 A		THR	A	138	-9.480	17.836	10.897	1.00
15	ATOM 16.63	1006 A	OG1 O	THR	Α	138	-8.271	17.308	10.321	1.00
	ATOM 17.63	1007 A		THR	Α	138	-9.308	3 19.330	10.788	1.00
20	ATOM 18.43	1008 A		THR	Α	138	-9.593	3 15.888	12.407	1.00
	ATOM 17.82	1009 A		THR	A	138	-8.662	2 15.296	12.954	1.00
	ATOM 18.06	1010 A	N N	THR	Α	139	-10.624	15.278	11.843	1.00
25	ATOM 17.69	1011 A	CA C	THR	A	139	-10.713	13.843	11.705	1.00
	ATOM 18.57	1012 A	CB C	THR	A	139	-12.020	13.472	10.947	1.00
30	ATOM 20.05	1013 A		THR	Α	139	-13.162	13.907	11.705	1.00
	ATOM 19.16	1014 A		THR	Α	139	-12.173	11.933	10.828	1.00

	ATOM 16.78	1015 A			A	139	-9.496	13.285	10.989	1.00
	ATOM 17.05	1016 A		THR	Α	139	-9.037	12.183	11.307	1.00
5	ATOM 15.81			ASP	A	140	-8.976	14.002	10.002	1.00
	ATOM 15.65	1018 A		ASP	Α	.140	-7.758	13.544	9.351	1.00
10				ASP	Α	14′0	-7.391	14.429	8.177	1.00
	ATOM 16.65	1020 A		ASP	Α	140	-8.279	14.209	6.984	1.00
	ATOM 18.76	1021 A		ASP	A	140	-8.495	15.189	6.263	1.00
15	ATOM 16.74			ASP	A	140	-8.781	13.102	6.702	1.00
		1023 A		ASP	Α	140	-6.567	13,.504	10.352	1.00
20	ATOM 15.72			ASP	A	140	-5.823	12.532	10.395	1.00
	ATOM 15.34	1025 A		SER	A	141	-6.395	14.555	11.133	1.00
	ATOM 15.53	1026 A		SER	A	141	-5.375	14.548	12.187	1.00
25	ATOM 14.57	1027 A		SER	Α	141	-5.428	15,823	13.006	1.00
	ATOM 16.14	1028 A	OG O	SER	Α	141	-5.275	16.936	12.173	1.00
30	ATOM 15.46		C C	SER	Α	141	-5.514	13.375	13.157	1.00
			0 0	SER	Α	141	-4.511	12.754	13.558	1.00

	ATOM 15.27			ARG	A	142	-6.754	13.100	13.546	1.00
•	ATOM 15.97			ARG	A	142	-7.053	11.998	14.462	1.00
5	ATOM 16.78			ARG	A	142	-8.539	12.004	14.843	1.00
		1034 A		ARG	A	142	-8.882	11.091	16.022	1.00
10	ATOM 22.40			ARG	A	142	-10.365	11.103	16.436	1.00
	ATOM 25.70			ARG	A	142	-10.533	10.384	17.704	1.00
	ATOM 29.38	1037 A		ARG	Α	142	-10.549	9.057	17.839	1.00
15		1038 A		ARG	Α	142	-10.423	8.249	16.786	1.00
	ATOM 30.56			ARG	Α	142	-10.685	8.524	19.048	1.00
20	ATOM 15.43			ARG	A	142	-6.703	10.643	13.860	1.00
	ATOM 14.36			ARG	Α	142	-6.107	9.778	14.534	1.00
	ATOM 14.96		N N	ASN	A	143	-7.068	10.437	12.593	1.00
25	ATOM 14.70	1043 A		ASN	A	143	-6.699	9.187	11.926	1.00
	ATOM 15.54	1044 A	CB C	ASN	A	143	-7.451	9.062	10.593	1.00
30	ATOM 16.85	1045 A	CG C	ASN	A	143	-8.952	8.709	10.803	1.00
	ATOM 20.66	1046 A	OD1 O	ASN	Α	143	-9.842	9.204	10.096	1.00

	ATOM 15.73			ASN	A	143	-9.206	7.828		1.00
	ATOM 15.26			ASN	A	143	-5.183	8.986	11.754	1.00
5	ATOM 15.15			ASN	A	143	-4.691	7.854	11.879	1.00
	ATOM 14.90			VAL	A	144	-4.438	10.060	11.450	1.00
10	ATOM 13.93			VAL	A	144	-2.976	9.987	11.467	1.00
	ATOM 14.08				A	144	-2.319	11.347	11.177	1.00
	ATOM 12.32			VAL	Α	144	-0.803	11.272	11.422	1.00
15	ATOM 13.08				Α	144	-2.625	11.818	9.748	1.00
	ATOM 14.23			VAL	A	144	-2.478	9.507	12.843	1.00
20	ATOM 13.96			VAL	A	144	-1.608	8.653	12.938	1.00
	ATOM 14.48			ASP	A	145	-3.021	10.077	13.916	1.00
	ATOM 14.49			ASP	A	145	-2.548	9.745	15.256	1.00
25	ATOM 14.81	1059 A	CB C	ASP	Α	145	-3.123	10.711	16.249	1.00
	ATOM 15.70	1060 · A	CG C	ASP	Α	145	-2.406	12.033	16.218	1.00
30	ATOM 14.69	1061 A	OD1 O	ASP	Α	145	-1.332	12.107	15.545	1.00
	ATOM 14.46	1062 A	OD2 O	ASP	A	145	-2.845	13.048	16.803	1.00

	ATOM 15.08	1063 A		ASP	A	145	-2.849	8.331	15.654	1.00
	ATOM 14.89	1064 A			A	145	-1.999	7.622	16.183	1.00
5	ATOM 15.66	1065 A			A	146	-4.065	7.906	15.361	1.00
	ATOM 15.98	1066 A		ASP	A	146	-4.470	6.545	15.608	1.00
10	ATOM 16.37			ASP	A	146	-5.931	6.400	15.184	1.00
	ATOM 17.81	1068 A		ASP	A	146	-6.565	5.107	15.705	1.00
	ATOM 18.17	1069 A		ASP	A	146	-6.337	4.735	16.879	1.00
15	ATOM 21.66	1070 A	OD2 O		A	146	-7.277	4.401	14.981	1.00
	ATOM 16.07	1071 A		ASP	A	146	-3.562	5.571	14.849	1.00
20	ATOM 16.60	1072 A		ASP	A	146	-3.047	4.607	15.408	1.00
	ATOM 15.73	1073 A		TYR	· <b>A</b>	147	-3.324	5.842	13.576	1.00
	ATOM 15.49			TYR	Α	147	-2.463	4.988	12.772	1.00
25	ATOM 15.22	1075 A		TYR	A	147	-2.387	5.486	11.314	1.00
	ATOM 16.31	1076 A		TYR	Α	147	-1.759	4.421	10.459	1.00
30	ATOM 17.35			TYR	A	147	-0.400	4.394	10.249	1.00
	ATOM 17.49			TYR	Α	147	0.180	3.380	9.506	1.00

•	ATOM 16.46	1079 A	CZ C	TYR A	147	-0.599	2.364	9.004	1.00
	ATOM 20.80	1080 A	OH O	TYR A	147	-0.022	1.354	8.281	1.00
5	ATOM 16.19	1081 A	CE2 C	TYR A	147	-1.944	2.346	9.227	1.00
	ATOM 16.98	1082 A		TYR A	147	-2.523	3.364	9.947	1.00
10	ATOM 15.68	1083 A		TYR A	147	-1.025	4.833	13.309	1.00
	ATOM 14.79	1084 A		TYR A	147	-0.491	3.719	13.385	1.00
	ATOM 16.33	1085 A	N N	VAL A	148	-0.399	5.953	13.652	1.00
15	ATOM 16.18	1086 A	CA C	VAL A	148	0.975	5.950	14.144	1.00
	ATOM 16.37	1087 A	CB C	VAL A	148	1.534	7.390	14.262	1.00
20	ATOM 17.53	1088 A		VAL A	148	2.953	7.397	14.909	1.00
	ATOM 16.39	1089 A		VAL A	148	1.600	8.044	12.899	1.00
	ATOM 16.59	1090 A	C C	VAL A	148	1.063	5.206	15.488	1.00
25	ATOM 16.63	1091 A	0 0	VAL A	148	2.022	4.481	15.765	1.00
	ATOM 16.70	1092 A	N N	ARG A	149	0.061	5.356	16.331	1.00
30	ATOM 18.28	1093 A	CA C	ARG A	149	0.109	4.628	17.589	1.00
	ATOM 18.33	1094 A	CB C	ARG A	149	-0.920	5.133	18.600	1.00

	ATOM 19.51			ARG	A	149	-0.	585	4.657	20.002	1.00
•	ATOM 20.84	1096 A	CD C	ARG	Α	149	-1.	566	5.035	21.071	1.00
5	ATOM 22.92	1097 A		ARG	Α	149	-0.	987	4.731	22.383	1.00
	ATOM 24.06	1098 A		ARG	A	149	-1.	661	4.491	23.504	1.00
10	ATOM 25.69	1099 A	NH1 N	ARG	A	149	-2.	985	4.521	23.538	1.00
	ATOM 23.61			ARG	A	149	-0.	987	4.221	24.616	1.00
	ATOM 18.63	1101 A		ARG	Α	149	-0.	035	3.126	17.382	1.00
15	ATOM 18.97	1102 A	0 0	ARG	A	149	0.	517	2.346	18.156	1.00
	ATOM 18.98	1103 A		LYS	A	150	-0.	739	2.720	16.326	1.00
20	ATOM 19.24			LYS	A	150	-0.	991	1.294	16.087	1.00
	ATOM 19.89	1105 A		LYS	_A	150	-2.	373	1.092	15.438	1.00
	ATOM 21.34	1106 A	CG C	LYS	A	150	-3.	576	1.358	16.389	1.00
25	ATOM 24.20	1107 A	CD C	LYS	Α	150	-4.	902	0.972	15.736	1.00
	ATOM 27.20	1108 A	CE C	LYS	A	150	-6.	136	1.437	16.531	1.00
30	ATOM 30.36	1109 A	NZ N	LYS	Α	150	-7.	373	1.614	15.668	1.00
	ATOM 18.99	1110 A	C C	LYS	À	150	0.	123	0.622	15.250	1.00

	ATOM 17.16			Α	150	0.296	-0.577	15.305	1.00
	ATOM 19.09	1112 A	N ASN N	A	151	0.916	1.407	14.526	1.00
5	ATOM 19.75		CA ASN	A	151	1.834	0.850	13.538	1.00
		1114 A	CB ASN	A	151	1.225	0.950	12.130	1.00
10	ATOM 19.86			Α	151	-0.141	0.299	12.025	1.00
	ATOM 19.33			A	151	-0.239	-0.905	11.855	1.00
	ATOM 19.31	1117 A		A	151	-1.198	1.090	12.167	1.00
15	ATOM		C ASN	A	151	3.150	1.599	13.557	1.00
	ATOM		O ASN	Α	151	3.193	2.807	13.793	1.00
20	ATOM 20.04	1120	N ASP	A	152	4.239	0.911	13.299	1.00
20	ATOM		CA ASP	A	152	5.508	1.595	13.319	1.00
			CB BASP	Α	152	6.571	0.640	13.830	0.35
25	ATOM	1123	CB AASP	Α	152	6.645	0.666	13.762	0.65
	21.56 ATOM	1124	CG BASP	A	152	6.199	0.067	15.205	0.35
	19.09 ATOM		CG AASP	Α	152	7.225	-0.117	12.631	0.65
30	23.76 ATOM 15.06		OD1BASP	A	152	5.318	0.654	15.901	0.35

	ATOM 27.77	1127 A		PΑ	152	6.404	-0.719	11.924	0.65
	ATOM 16.81		OD2BAS	PΑ	152	6.703	-0.977	15.653	0.35
5	ATOM 27.40	1129 A	OD2AAS	PΑ	152	8.471	-0.170	12.353	0.65
		1130 A		SP A	. 152	5.822	2.270	11.959	1.00
10	ATOM 20.60	1131 A		SP A	. 152	6.748	1.916	11.253	1.00
	ATOM 16.58	1132 A	N ME	ET A	153	4.988	3.250	11.628	1.00
	ATOM 16.03	1133 A	CA ME	T A	153	5.154	4.050	10.437	1.00
15	ATOM 16.23	1134 A		ТА	153	3.876	4.007	9.619	1.00
		1135 A	CG ME	ТА	153	3.885	4.921	8.432	1.00
20	ATOM 21.72	1136 A		т А	153	4.694	4.182	7.030	1.00
		1137 A		ΤА	153	3.290	3.549	6.297	1.00
	ATOM 14.80	1138 A		T A	153	5.443	5.482	10.871	1.00
25		1139 A		T A	153	4.684	6.058	11.646	1.00
	ATOM 13.34	1140 A		R A	154	6.525	6.059	10.368	1.00
30	ATOM 13.08			R A	154	6.813	7.482	10.638	1.00
	ATOM 13.02			R A	154	8.324	7.699	10.652	1.00

	ATOM 11.51		OG1 O	THR	Α	154		8.886	6.949	11.724	1.00
	ATOM 14.36	1144 A	CG2 C	THR	A	154	,	8.693	9.145	10.963	1.00
5	ATOM 12.50	1145 A		THR	A	154		6.153	8.310	9.573	1.00
	ATOM 12.64	1146 A		THR	A	154		6.396	8.108	8.371	1.00
10	ATOM 12.34		N N	ILE	A	155		5.290	9.227	9.987	1.00
	ATOM 13.00	1148 A		ILE	A	155		4.492	10.002	9.037	1.00
	ATOM 13.05	1149 A		ILE	Α	155		2.983	9.799	9.346	1.00
15	ATOM 13.73	1150 A		ILE	Α	155		2.637	8.307	9.279	1.00
	ATOM 12.93	1151 A		ILE	A	155		1.121	8.017	9.274	1.00
20	ATOM 13.58	1152 A		ILE	A	155		2.121	10.578	8.371	1.00
	ATOM 13.01	1153 A		ILE	A	155		4.861	11.480	9.137	1.00
	ATOM 12.79	1154 A	0 0	ILE	Α	155		4.894	12.038	10.233	,1.00
25	ATOM 12.16	1155 A	N N	LEU	A	156		5.125	12.117	8.001	1.00
	ATOM 12.88	1156 A	CA C	LEU	Α	156		5.509	13.528	7.982	1.00
30	ATOM 12.18	1157 A		LEU	A	156		6.903	13.692	7.354	1.00
	ATOM 13.25	1158 A	CG C	LEU	A	156		8.089	12.960	8.007	1.00

		1159 A		LEU	A	156	8.365	11.607	7.326	1.00
		1160 A		LEU	A	156	9.339	13.796	7.910	1.00
5	ATOM 13.49			LEU	A	156	4.485	14.328	7.192	1.00
		1162 A		LEU	A	156	3.982	13.850	6.160	1.00
10	ATOM 12.79			PHE	A	157	4.197	15.540	7.659	1.00
	ATOM 13.07			PHE	A	157	3.282	16.451	7.003	1.00
	ATOM 13.62			PHE	A	157	1.938	16.564	7.772	1.00
15		1166 A		PHE	A	157	0.957	15.504	7.401	1.00
	ATOM 11.22			PHE	A	157	0.191	15.636	6.272	1.00
20	ATOM 14.22			PHE	Α	157	-0.678	14.632	5.896	1.00
	ATOM 14.61			PHE	A	157	-0.743	13.441	6.630	1.00
	ATOM 15.64			PHE	Α	157	0.013	13.296	7.743	1.00
25		1171 A		PHE	Α,	157	0.891	14.312	8.122	1.00
	ATOM 13.18	1172 A	C C	PHE	A	157	3.899	17.852	6.928	1.00
30	ATOM 12.04	1173 A	0 0	PHE	A	157	4.527	18.318	7.867	1.00
	ATOM 13.46	1174 A	N N	ALA	A	158	3.700	18.500	5.793	1.00

	ATOM 13.31			ALA	A	158	3.958	19.921	5.623	1.00
	ATOM 14.02				A	158	3.509	20.334	4.235	1.00
5	ATOM 13.75				A	158	3.181	20.703	6.672	1.00
	ATOM 13.75	1178 A			A	158	2.031	20.380	6.965	1.00
10	ATOM 13.45				A	159	3.787	21.752	7.215	1.00
	ATOM 13.81				A	159	3.122	22.582	8.210	1.00
	ATOM 13.64				A	159	4.151	23.495	8.944	1.00
15	ATOM 14.14				Α	159	2.043	23.473	7.628	1.00
	ATOM 14.00				Α	159	1.175	23.924	8.364	1.00
20	ATOM 15.19				Α	160	2.131	23.753	6.330	1.00
	ATOM 15.34			GLY	Α	160	1.230	24.680	5.652	1.00
	ATOM 14.93		C C	GLY	Α	160	1.957	25.941	5.236	1.00
25	ATOM 14.62		0 0	GLY	A	160	3.041	26.238	5.736	1.00
	ATOM 15.04	1188 A	N N	ASN	Α	161	1.371	26.686	4.307	1.00
30	ATOM 15.84	1189 A	CA C	ASN	A	161	1.983	27.902	3.789	1.00
	ATOM 15.91	1190 A		ASN	A	161	2.072	27.872	2.261	1.00

	ATOM 17.40			ASN	A	161	3.048	26.851	1.712	1.00
	ATOM 21.70			ASN	A	161	3.001	26.550	0.490	1.00
5	ATOM 11.15	1193 A		ASN	A	161	3.888	26.267	2.569	1.00
		1194 A		ASN	A	161	1.131	29.114	4.123	1.00
10	ATOM 17.07			ASN	A	161	0.956	29.965	3.286	1.00
	ATOM 18.36			GLU	A	162	0.575	29.179	5.324	1.00
	ATOM 18.85	1197 A		GLU	A	162	-0.392	30.213	5.668	1.00
15	ATOM 19.64			GLU	A	162	-1.672	29.537	6.211	1.00
		1199 A		GLU	A	162	-2.431	28.723	5.150	1.00
20	ATOM 26.12	1200 A		GLU	A	162	-1.756	27.381	4.788	1.00
	ATOM 28.48	1201 A		GLU	A	162	-1.585	26.545	5.702	1.00
		1202 A		GLU	A	162	-1.405	27.149	3.590	1.00
25	ATOM 19.39	1203 A		GLU	A	162	0.147	31.262	6.657	1.00
	ATOM 18.80	1204 A		GLU	Α	162	-0.633	32.031		1.00
30	ATOM 19.39	1205 A		GLY	A	163	1.472	31.338	6.820	1.00
,	ATOM 20.03		CA	GLY	A	163	2.082	32.322	7.705	1.00

	ATOM 21.41	1207 A		GLY	A	163	2.224	33.699	7.048	1.00
	ATOM 20.72			GLY	A	163	1.822	33.866	5.877	1.00
5	ATOM 21.93			PRO	A	164	2.835	34.671	7.737	1.00
	ATOM 22.22	1210 A		PRO	A	164	3.496	34.491	9.053	1.00
10	ATOM 22.99			PRO	A	164	4.575	35.577	9.050	1.00
	ATOM 23.13			PRO	A	164	3.945	36.720	8.171	1.00
	ATOM 22.03	1213 A		PRO	A	164	2.976	36.047	7.209	1.00
15		1214 A		PRO	Α	164	2.681	34.621	10.329	1.00
	ATOM 21.36			PRO	Α	164	3.289	34.603	11.414	1.00
20	ATOM 21.66			GLY	A	165	1.363	34.702	10.239	1.00
	ATOM 21.84	1217 A		GLY	A	165	0.537	34.844	11.414	1.00
	ATOM 22.27	1218 A		GLY	A	165	0.522	33.581	12.243	1.00
25	ATOM 22.20	1219 A		GLY	A	165	0.680	32.440	11.713	1.00
	ATOM 22.06	1220 A		SER	A	166	0.305	33.762	13.543	1.00
30	ATOM 21.96	1221 A	CA C	SER	A	166	0.290	32.645	14.470	1.00
	ATOM 23.25	1222 A		SER	A	166	0.344	33.167	15.917	1.00

	ATOM 25.13	1223 A		SER	A	166	-0.948	33.579	16.367	1.00
	ATOM 21.45			SER	A	166	-0.954	31.807	14.241	1.00
5	ATOM 21.15			SER	Α	166	-1.949	32.311	13.716	1.00
	ATOM 20.07		N N	GLY	Α	167	-0.879	30.515	14.574	1.00
10	ATOM 19.63	1227 A		GLY	A	167	-2.032	29.639	14.548	1.00
	ATOM 19.18			GLY	A	167	-2.478	29.248	13.140	1.00
	ATOM 18.57			GLY	A	167	-3.652	29.051	12.911	1.00
15		1230 A		THR	A	168	-1.541	29.140	12.200	1.00
	ATOM 17.13			THR	Α	168	-1.893	28.857	10.810	1.00
20	ATOM 17.32			THR	A	168	-1.295	29.958	9.908	1.00
	ATOM 14:44			THR	A	168	0.077	30.172	10.261	1.00
	ATOM 17.60	1234 A		THR	A	168	-1.988	31.299	10.156	1.00
25	ATOM 16.75			THR	A	168	-1.496	27.465	10.306	1.00
		1236 A		THR	A	168	-1.462	27.213	9.091	1.00
30	ATOM 15.95			ILE	A	169	-1.265	26.540	11.234	1.00
		1238 A		ILE	A	169	-0.863	25.191	10.871	1.00

	ATOM 15.09	1239 A		ILE A	169	-0.454	24.378	12.127	1.00
	ATOM 14.88	1240 A		ILE A	169	0.626	25.109	12.942	1.00
5	ATOM 16.38	1241 · A		ILE A	169	2.021	25.201	12.267	1.00
		1242 A		ILE A	169	0.021	22.988	11.720	1.00
10		1243 A		ILE A	169	-2.004	24.477	10.137	1.00
	ATOM 14.50	1244 A		ILE A	169	-3.146	24.470	10.590	1.00
	ATOM 14.94	1245 A		SER A	170	-1.681	23.857	9.018	1.00
15	ATOM 15.41	1246 A		SER A	170	-2.665	23.060	8.310	1.00
		1247 A		SER A	170	-2.299	23.004	6.821	1.00
20	ATOM 16.03	1248 A		SER A	170	-1.040	22.404	6.585	1.00
		1249 A		SER A	170	-2.855	21.660	8.904	1.00
	ATOM 13.80	1250 A		SER A	170	-1.986	21.137	9.616	1.00
25	ATOM 14.65	1251 A	N N	ALA A	171	-3.992	21.036	8.582	1.00
	ATOM 14.75	1252 A	CA C	ALA A	171	-4.244	19.651	8.933	1.00
30	ATOM 15.62		CB C	ALA A	171	-5.700	19.507	9.443	1.00
	ATOM 15.02		C C	ALA A	171	-4.043	18.750	7.740	1.00

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	ATOM 14.12	1255 A			. A	171	-4.475	19.096	6.652	1.00
	ATOM 15.48				A	172	-3.482	17.548	7.899	1.00
5	ATOM 15.17				Α	172	-3.078	16.913	9.167	1.00
		1258 A		PRO	Α	172	-3.080	15.411	8.796	1.00
10	ATOM 15.73	1259 A		PRO	A	172	-3.707	15.336	7.456	1.00
	ATOM 15.43			PRO	A	172	-3.401	16.614	6.768	1.00
		1261 A			A	172	-1.724	17.260	9.788	1.00
15		1262 A		PRO	A	172	-1.284	16.499	10.651	1.00
		1263 A		GLY	Α	173	-1.086	18.352	9.382	1.00
20		1264 A		GLY	A	173	0.078	18.895	10.064	1.00
				GLY	A	173	-0.158	19.147	11.553	1.00
	ATOM 14.08	1266 A		GLY	A	173	0.809	19.174	12.339	1.00
25	ATOM 13.50		N N	THR	Α	174	-1.419	19.291	11.956	1.00
	ATOM 13.19	1268 A	CA C	THR	Α	174	-1.758	19.475	13.375	1.00
30		1269 A	CB C	THR	Α	174	-3.137	20.125	13.530	1.00
		1270 A		THR	A	174	-4.104	19.394	12.743	1.00

	ATOM 14.22	1271 A		THR		174	-3.114	21.510	12.957	1.00
		1272 A		THR	Α	174	-1.774	18.188	14.172	1.00
5	ATOM 12.08			THR	Α	174	-1.909	18.227	15.390	1.00
	ATOM 12.94	1274 A		ALA	A	175	-1.696	17.040	13.505	1.00
10	ATOM 12.90			ALA	Α	175	-1.614	15.772	14.213	1.00
		1276 A		ALA	Α	175	-1.422	14.641	13.211	1.00
	ATOM 12.44	1277 A			Α	175	-0.484	15.740	15.264	1.00
15		1278 A		ALA	Α	175	0.601	16.233	15.043	1.00
	ATOM 13.08	1279 A		LYS	Α	176	-0.739	15.131	16.398	1.00
20	ATOM 13.00	1280 A		LYS	Α	176	0.269	15.057	17.466	1.00
		1281 A		LYS	Α	176	-0.383	14.511	18.719	1.00
	ATOM 13.87	1282 A	CG C	LYS	Α	176	-1.406	15.392	19.366	1.00
25	ATOM 15.77	1283 A		LYS	Α	176	-2.044	14.693	20.553	1.00
	ATOM 16.63	1284 A	CE . C	LYS	Α	176	-3.179	13.722	20.173	1.00
30	ATOM 16.58	1285 A	NZ N	LYS	Α	176	-3.738	13.048	21.388	1.00
	ATOM 13.10	1286 A	C C	LYS	Α	176	1.433	14.107	17.115	1.00

	ATOM 12.98	1287 A	LYS	A	176	2.559	14.289	17.538	1.00
	ATOM 12.81	1288 A	ASN	A	177	1.119	13.047	16.390	1.00
5	ATOM 12.78	1289 A	ASN	A	177	2.047	11.933	16.187	1.00
		1290 A	ASN	A	177	1.278	10.628	16.301	1.00
10	ATOM 12.12	1291 A	ASN	Α	177	0.733	10.382	17.718	1.00
		1292 A	ASN	A	177	1.135	11.043	18.682	1.00
	ATOM 10.81	1293 A	ASN	A	177	-0.179	9.416	17.844	1.00
15	ATOM 12.68	1294 A	ASN	Α	177	2.822	11.966	14.876	1.00
		1295 A	ASN	Α	177	3.692	11.097	14.621	1.00
20	ATOM 12.80	1296 A	ALA	Α	178	2.483	12.933	14.029	1.00
		1297 A	ALA	A	178	3.234	13.208	12.801	1.00
		1298 A	ALA	A	178	2.382	13.938	11.817	1.00
25		1299 A	ALA	A	178	4.439	14.052	13.141	1.00
		1300 A	ALA	A	178	. 4.471	14.685	14.188	1.00
30	ATOM 11.71		ILE	A	179	5.458	13.985	12.293	1.00
	ATOM 11.72	1302 A		A	179	6.531	14.966	12.283	1.00

	ATOM 11.54	1303 A		ILE	Α	179	7.838	14.364	11.812	1.00
		1304 A		ILE	A	179	8.251	13.222	12.712	1.00
5	ATOM 14.82	1305 A		ILE	A	179	9.472	12.467	12.196	1.00
		1306 A		ILE	A	179	8.927	15.437	11.783	1.00
10	ATOM 11.98			ILE	A	179	6.085	16.076	11.317	1.00
		1308 A		ILE	A	179	5.943	15.852	10.109	1.00
	ATOM 11.27	1309 A		THR	Α	180	5.813	17.248	11.871	1.00
15	ATOM 11.76	1310 A		THR	A	180	5.357	18.383	11.074	1.00
	ATOM 11.79			THR	A	180	4.260	19.120	11.818	1.00
20	ATOM 12.06	1312 A		THR	A	180	3.166	18.214	12.084	1.00
	ATOM 12.72	1313 A		THR	A	180	3.603	20.224	10.929	1.00
	ATOM 11.82			THR	A	180	6.530	19.306	10.690	1.00
25	ATOM 11.02	1315 A		THR	A	180	7.286	19.762	11.533	1.00
•	ATOM 11.42	1316 A		VAL	Α	181	6.662	19.590	9.401	1.00
30	ATOM 11.43	1317 A	CA C	VAL	Α	181	7.830	20.305	8.899	1.00
		1318 A		VAL	Α	181	8.492	19.464	7.814	1.00

	ATOM 12.42	1319 A	VAL	A	181	9.744	20.118	7.309	1.00
	ATOM 12.33	1320 A	VAL	A	181	8.757	18.055	8.351	1.00
5	ATOM 11.62	1321 A	VAL	Α	181	7.511	21.680	8.302	1.00
	ATOM 12.16	1322 A	VAL	A	181	6.667	21.800	7.399	1.00
10		1323 A	GLY	A	182	8.187	22.704	8.812	1.00
	ATOM 12.80		GLY	Α	182	8.095	24.042	8.273	1.00
		1325 A	GLY	A	182	9.296	24.352	7.391	1.00
15	ATOM 14.13		GLY	A	182	10.243	23.574	7.344	1.00
		1327 A	ALA	A	183	9.264	25.492	6.700	1.00
20	ATOM 14.22	1328 A	ALA	Α	183	10.312	25.837	5.776	1.00
	ATOM 14.53	1329 A	ALA	A	183	9.709	26.166	4.401	1.00
	ATOM 14.32		ALA	A	183	11.205	27.001	6.238	1.00
25	ATOM 14.13		ALA	Α	183	10.717	28.110	6.498	1.00
	ATOM 14.17	1332 A	THR	Α	184	12.512	26.737	6.293	1.00
30	ATOM 14.33	1333 A	THR	Α	184	13.513	27.799	6.294	1.00
	ATOM 14.19		THR	Α	184	14.743	27.451	7.159	1.00

	ATOM	1335	OG1	THR	Α	184	15,180	26.103	6.925	1.00
	13.83	A								
	ATOM 13.70	1336 A		THR	Α	184	14.383	27.474	8.636	1.00
5	ATOM 15.47	1337 A		THR	Α	184	13.905	28.018	4.841	1.00
	ATOM 15.87			THR	Α	184	13.380	27.354	3.934	1.00
10	ATOM 15.13	1339 A		GLU	A	185	14.861	28.919	4.618	1.00
	ATOM 14.03			GLU	A	185	15.328	29.246	3.290	1.00
	ATOM 13.82	1341 A		GLU	A	185	15.696	30.766	3.230	1.00
15	ATOM 15.09	1342 A		GLU	A	185	14.492	31.673	3.495	1.00
	ATOM 14.09	1343 A		GLU	A	185	14.785	33.172	3.329	1.00
20	ATOM 15.60			GLU	Α	185	15.911	33.541	2.985	1.00
		1345 A	•	GLU	A	185	13.871	33.984	3.528	1.00
	ATOM 13.70	1346 A	C C	GLU	A	185	16.511	28.376	2.863	1.00
25	ATOM 14.17	1347 A	0 0	GLU	A	185	17.387	28.011	3.675	1.00
	ATOM 12.64	1348 A	N N	ASN	A	186	16.521	28.008	1.587	1.00
30	ATOM 13.44	1349 A	CA C	ASN	A	186	17.707	27.452	0.959	1.00
	ATOM 13.84	1350 A	CB C	ASN	Α	186	17.345	26.758	-0.353	1.00

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	ATOM 14.82	1351 A	CG C	ASN	A	186	·	18.293	25.630	-0.717	1.00
	ATOM 14.62	1352 A	OD1 O	ASN	Α	186		19.084	25.169	0.099	1.00
5	ATOM 15.51	1353 A	ND2 N	ASN	A	186		18.189	25.156	-1.970	1.00
	ATOM 13.83	1354 A		ASN	A	186		18.652	28.603	0.681	1.00
· 10	ATOM 14.50	1355 A		ASN	A	186		18.244	29.769	0.711	1.00
	ATOM 14.83	1356 A	N N	LEU	Α	187		19.920	28.298	0.470	1.00
	ATOM 14.62	1357 A	CA C	LEU	A	187		20.892	29.352	0.213	1.00
15	ATOM 15.48	1358 A	CB C	LEU	A	187		22.144	29.144	1.018	1.00
	ATOM 17.25	1359 A	CG C	LEU	A	187		23.144	30.319	0.975	1.00
20	ATOM 18.56	1360 A		LEU	A	187		22.504	31.587	1.469	1.00
	ATOM 20.46	1361 A		LEU	A	187		24.394	29.973	1.816	1.00
	ATOM 14.80	1362 A	C C	LEU	Α	187		21.205	29.360	-1.279	1.00
`25	ATOM 14.07	1363 A	0 0	LEU	A	187		22.106	28.692	-1.734	1.00
	ATOM 15.63	1364 A	N N	ARG	A	188		20.398	30.083	-2.023	1.00
30	ATOM 17.55	1365 A	CA C	ARG	A	188		20.631	30.308	-3.454	1.00
	ATOM 17.02	1366 A	CB C	ARG	Α	188		19.658	29.484	-4.273	1.00

	ATOM 17.82	1367 A	CG C	ARG	A	188		19.842	27.989	-4.168	1.00
	ATOM 19.96	1368 A	CD C	ARG	A	188		19.063	27.213	-5.267	1.00
5	ATOM 18.26	1369 A	NE N	ARG	A	188		19.315	25.782	-5.224	1.00
	ATOM 19.52	1370 A	CZ C	ARG	Α	188		20.339	25.172	-5.814	1.00
10	ATOM 17.91	1371 A	NH1 N	ARG	Α	188		21.235	25.846	-6.530	1.00
	ATOM 19.41	1372 A	NH2 N	ARG	A	188		20.475	23.867	-5.693	1.00
	ATOM 17.89	1373 A	C C	ARG	A	188		20.387	31.804	-3.694	1.00
15	ATOM 18.33	1374 A	0	ARG	A	188		19.379	32.189	-4.251	1.00
	ATOM 19.58	1375 A	N N	PRO	A	189		21.273	32.646	-3.181	1.00
20	ATOM 20.68	1376 A	CA C	PRO	A	189		20.990	34.082	-3.061	1.00
	ATOM 21.07	1377 A	CB	PRO	Α	189		22.179	34.613	-2.239	1.00
	ATOM 21.15	1378 A	CG C	PRO	A	189	-	23.271	33.608	-2.417	1.00
25	ATOM 20.12	1379 A	CD C	PRO	A	189		22.599	32.288	-2.657	1.00
	ATOM 21.39	1380 A	C C	PRO	Α	189		20.833	34.863	-4.373	1.00
30	ATOM 20.51	1381 A	0 0	PRO	A	189		20.276	35.975	-4.347	1.00
	ATOM 22.89	1382 A		SER	Α	190		21.285	34.307	-5.492	1.00

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	ATOM 24.65			SER	A	190	21.033	34.940	-6.796	1.00
	ATOM 24.76	1384 A		SER	A	190	21.685	34.135	-7.932	1.00
5	ATOM 25.85	1385 A		SER	A	190	21.082	32.831	-8.046	1.00
	ATOM 25.23			SER	A	190	19.525	35.098	-7.028	1.00
10	ATOM 26.47				A	190	19.080	35.918	-7.850	1.00
	ATOM 25.36	1388 A		PHE	A	191	18.723	34.365	-6.258	1.00
	ATOM 25.28	1389 A	CA C	PHE	A	191	17.264	34.446	-6.389	1.00
15	ATOM 25.00		CB C	PHE	A	191	16.643	33.046	-6.156	1.00
	ATOM 23.34			PHE	A	191	16.841	32.089	-7.310	1.00
20	ATOM 21.81	1392 A		PHE	A	191	17.565	30.932	-7.159	1.00
		1393 A		PHE	A	191	17.735	30.052	-8.218	1.00
1	ATOM 21.46	1394 A		PHE	Α	191	17.180	30.341	-9.470	1.00
25	ATOM 22.61	1395 A	CE2 C	PHE	Α	191	16.449	31.484	-9.631	1.00
	ATOM 25.47	1396 A	CD2 C	PHE	A	191	16.288	32.361	-8.562	1.00
30	ATOM 25.71	1397 A	C C	PHE	A	191	16.388	35.561	-5.720	1.00
	ATOM 27.33	1398 A	0 0	PHE	Ą	191	15.184	35.500	-5.877	1.00

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	ATOM 26.98	1399 . A			A	192		16.823	36.552	-4.944	1.00
	ATOM 26.29	1400 A	CA C	GLY	Α	192		17.639	36.484	-3.783	1.00
5	ATOM 25.37	1401 A		GLY	A	192		16.795	36.445	-2.478	1.00
	ATOM 25.24	1402 A		GLY	A	192		17.008	35.528	-1.733	1.00
10	ATOM 24.49			SER	A	193		15.858	37.355	-2.179	1.00
	ATOM 24.39	1404 A		SER	Α	193		15.332	37.444	-0.778	1.00
	ATOM 24.51	1405 A		SER	A	193		14.452	38.689	-0.554	1.00
15	ATOM 25.19	1406 A		SER	A	193		13.058	38.407	-0.623	1.00
	ATOM 23.94			SER	Α	193		14.664	36.176	-0.133	1.00
20	ATOM 22.27	1408 A		SER	Α	193		14.740	35.973	1.085	1.00
	ATOM 23.39	1409 A		TYR	A	194	·	14.037	35.331	-0.949	1.00
	ATOM 23.08			TYR	A	194		13.497	34.046	-0.477	1.00
25	ATOM 23.87	1411 A		TYR	A	194		12.407	33.559	-1.439	1.00
	ATOM 27.80	1412 A		TYR	A	194		11.044	34.129	-1.144	1.00
30	ATOM 31.12	1413 · A		TYR	A	194		10.563	35.240	-1.832	1.00
	ATOM 32.91	1414 <sub>.</sub> A	CE1 C	TYR	Α	194		9.317	35.775	-1.554	1.00

	ATOM 34.12	1415 A		TYR	A	194	8.52	35.182	-0.591	1.00
	ATOM 38.22			TYR	A	194	7.28	35.696	-0.311	1.00
5	ATOM 33.28	1417 A		TYR	A	194	8.974	34.076	0.108	1.00
		1418 A		TYR	A	194	10.229	33.556	-0.169	1.00
10	ATOM 21.59			TYR	Α	194	14.54	32.930	-0.289	1.00
		1420 A		TYR	A	194	14.225	31.848	0.236	1.00
	ATOM 20.44				A	195	15.78	33.185	-0.695	1.00
15		1422 A		ALA	A	195	16.838	32.181	-0.610	1.00
		1423 A		ALA	A	195	16.915	31.365	-1.892	1.00
20	ATOM 19.93			ALA	A	195	18.222	32.757	-0.270	1.00
		1425 A		ALA	A	195	19.230	32.354	-0.877	1.00
	ATOM 19.15	1426 A	N N	ASP	A	196	18.264	33.615	0.750	1.00
25	ATOM 19.86	1427 A	CA C	ASP	A	196	19.472	34.355	1.126	1.00
	ATOM 20.04	1428 A	CB C	ASP	A	196	19.264	35.861	0.919	1.00
30	ATOM 22.11	1429 A	CG C	ASP	A	196	18.198	36.453	1.814	1.00
	ATOM 23.87	1430 A	OD1 O	ASP	A	196	18.040	37.693	1.696	1.00

		1431 A		ASP	Α	196	17.461	35.822	2.649	1.00
•	ATOM 19.90			ASP	A	196	20.025	34.163	2.549	1.00
5	ATOM 19.61	1433 A			A	196	21.092	34.705	2.869	1.00
	ATOM 18.85				A	197	19.326	33.410	3.394	1.00
10	ATOM 18.29			ASN	A	197	19.790	33.177	4.757	1.00
	ATOM 18.68				A	197	19.410	34.369	5.644	1.00
	ATOM 19.48	1437 A		ASN	A	197	20.123	34.360	7.001	1.00
15		1438 A		ASN	A	197	20.221	33.319	7.630	1.00
	ATOM 14.55			ASN	A	197	20.603	35.541	7.455	1.00
20	17.30			ASN	A	197	19.198	31.861	5.304	1.00
		1441 A		ASN	A	197	17.986	31.734	5.463	1.00
	ATOM 16.67		N N	ILE	A	198	20.066	30.901	5.608	1.00
25	ATOM 16.04	1443 A	CA C	ILE	A	198	19.606	29.557	5.993	1.00
	ATOM 15.64	1444 A	CB C	ILE	Α	198	20.771	28.571	6.020	1.00
30	ATOM 16.27	1445 A	CG1 C	ILE		198	21.724	28.885	7.179	1.00
	ATOM 18.08	1446 A		ILE	A	198	22.734	27.781	7.490	1.00

	ATOM 16.50	1447 A	ILE	A	198	21.459	28.530	4.679	1.00
	ATOM 15.03		ILE	A	198	18.897	29.560	7.352	1.00
5	ATOM 15.12		ILE	A	198	18.222	28.605	7.723	1.00
	ATOM 14.78		ASN	A	199	19.054	30.642	8.102	1.00
10	ATOM 14.68		ASN	A	199	18.316	30.794	9.344	1.00
	ATOM 14.98		ASN	A	199	19.180	31.609	10.332	1.00
	ATOM 15.69		ASN	A	199	20.487	30.948	10.708	1.00
15		1454 A	ASN	A	199	20.560	29.757	10.907	1.00
	ATOM 20.04		ASN	A	199	21.526	31.768	10.903	1.00
20	ATOM 14.49		ASN	A	199	17.036	31.597	9.311	1.00
	ATOM 14.69		ASN	A	199	16.239	31.490	10.227	1.00
	ATOM 15.73		HIS	Α	200	16.736	32.328	8.241	1.00
25	ATOM 14.99		HIS	A	200	15.375	32.648	7.854	1.00
	ATOM 15.17		HIS	Α	200	15.338	33.612	6.641	1.00
30	ATOM 17.24		HIS	A	200	16.005	34.942	6.871	1.00
	ATOM 16.94		HIS	A	200	16.242	35.840	5.842	1.00

		1463 A		HIS	A	200	16.842	36.916	6.327	1.00
	ATOM		NE2	HIS	A	200	17.009	36.751	7.628	1.00
5		1465 A		HIS	Α	200	16.469	35.538	7.999	1.00
		1466 A		HIS	A	200	14.327	31.581	7.730	1.00
10	ATOM 14.41			HIS	A	200	14.472	30.673	6.965	1.00
		1468 A			A	201	13.251	31.772	8.496	1.00
	ATOM 16.37			VAL	Α	201	12.004	31.059	8.294	1.00
15		1470 A		VAL	A	201	11.103	31.185	9.523	1.00
		1471 A		VAL	Α	201	9.780	30.428	9.297	1.00
20	ATOM 18.01			VAL	A	201	11.841	30.668	10.783	1.00
		1473 A			Α	201	11.313	31.683	7.089	1.00
	ATOM 17.09	1474 A	0 0	VAL	A	201	11.250	32.900	6.973	1.00
25	ATOM 17.70	1475 A	N N	ALA	Α	202	10.872	30.865	6.143	1.00
	ATOM 17.52	1476 A	CA C	ALA	Α	202	10.233	31.396	4.949	1.00
30	ATOM 18.76	1477 A	CB C	ALA	Α	202	9.859	30.265	4.018	1.00
	ATOM 17.84	1478 A	C C	ALA	A	202	9.000	32.169	5.383	1.00

		1479 A		A 202	8.263	31.734	6.263	1.00
	ATOM 18.20	`1480 A	n GLN N	A 203	8.770	33.332	4.783	1.00
5		1481 A		A 203	7.629	34.135	5.192	1.00
			CB BGLN Z	A 203	7.542	35.347	4.260	0.40
10		1483 A		A 203	7.529	35.467	4.445	0.60
	ATOM 22.36			A 203	7.527	36.681	4.943	0.40
	ATOM 24.58			A 203	6.748	36.514	5.261	0.60
15	ATOM 25.52	1486 A		A 203	6.379	37.556	4.452	0.40
-	ATOM 28.39	1487 A		A 203	7.553	37.090	6.439	0.60
20	ATOM 27.97		OE1BGLN A	203	5.568	37.122	3.624	0.40
	ATOM 33.69		OE1AGLN A	203	8.525	37.816	6.236	0.60
,	ATOM 24.61			. 203	6.299	38.772	4.972	0.40
25	ATOM 31.16			203	7.155	36.751	7.655	0.60
	ATOM 18.58	1492 A	C GLN A	A 203	6.291	33.391	5.152	1.00
30	ATOM 18.67	1493 A	O GLN A	A 203	5.458	33.580	6.028	1.00
	ATOM 17.22	1494 A	N PHE A	204	6.090	32,533	4.163	1.00

	ATOM 16.75			PHE	A	204		4.805	31.833	4.027	1.00
	ATOM 16.25	1496 A		PHE	Α	204	•	4.603	31.335	2.589	1.00
5	ATOM 16.52			PHE	Α	204		5.720	30.475	2.093	1.00
	ATOM 16.66	1498 A		PHE	A	204		5.857	29.158	2.526	1.00
10	ATOM 17.13	1499 A		PHE	A	204		6.893	28.378	2.083	1.00
	ATOM 14.67	1500 A		PHE	A	204		7.854	28.909	1.234	1.00
	ATOM 16.10	1501 A		PHE	A	204		7.747	30.231	0.816	1.00
15	ATOM 15.39	1502 . A		PHE	Α	204		6.693	31.009	1.267	1.00
	ATOM 16.21	1503 A		PHE	Α	204		4.670	30.647	5.018	1.00
20	ATOM 15.42			PHE	A	204		3.570	30.150	5.198	1.00
	ATOM 15.36	1505 A		SER	A	205		5.754	30.223	5.688	1.00
		1506 A	CA C	SER	Α	205		5.692	28.983	6.508	1.00
25	ATOM 15.27	1507 A		SER	Α	205		7.068	28.579	7.063	1.00
	ATOM 15.10	1508 A	OG O	SER	Α	205		7.042	27.254	7.585	1.00
30	ATOM 14.84	1509 A	C C	SER	Α	205		4.657	29.103	7.615	1.00
	ATOM 16.26	1510 A	0 0	SER	Α	205		4.618	30.092	8.319	1.00

	ATOM 15.82	1511 A			A	206	3.764	28.141	7.753	1.00
	ATOM 15.73	1512 A	CA C	SER	A	206	2.751	28.237	8.818	1.00
5	ATOM 16.10	1513 A			A	206	1.714	-27.117	8.735	1.00
		1514 A			A	206	0.811	27.350	7.655	1.00
10	ATOM 15.92	1515 A		SER	A	206	3.421	28.221	10.186	1.00
	ATOM 15.30				A	206	4.486	27.589	10.362	1.00
	ATOM 15.72	1517 A			Α	207	2.786	28.928	11.113	1.00
15	ATOM 16.34	1518 A		ARG	A	207	3.289	29.140	12.455	1.00
	ATOM 16.50			ARG	A	207	3.511	30.636	12.715	1.00
20	ATOM 18.52	1520 A		ARG	A	207	4.189	31.375	11.542	1.00
•	ATOM 20.29	1521 A		ARG	A	207	5.604	30.916	11.227	1.00
	ATOM 22.13			ARG	A	207	6.146	31.519	10.012	1.00
25	ATOM 22.20	1523 A		ARG	Å	207	6.821	32.643	9.981	1.00
	ATOM 25.41	1524 A	NH1 N	ARG	Α	207	7.056	33.294	11.080	1.00
30	ATOM 24.08	1525 A		ARG	Α	207	7.256	33.124	8.838	1.00
	ATOM 15.97	1526 A		ARG	A	207	2.330	28.556	13.471	1.00

	ATOM 15.01	1527 A		ARG	A	207		1.096	28.605	13.301	1.00
	ATOM 15.16	1528 A	N N	GLY	A	208		2.903	27.974	14.521	1.00
5	ATOM 16.14	1529 A		GLY	A	208		2.139	27.523	15.655	1.00
	ATOM 16.50	1530 A		GLY	A	208		1.622	28.688	16.476	1.00
10	ATOM 17.36			GLY	A	208		1.753	29.830	16.059	1.00
	ATOM 17.42				A	209		0.999	28.423	17.617	1.00
	ATOM 17.56	1533 A		PRO	A	209		0.727	27.067	18.089	1.00
15		1534 A		PRO	A	209		0.407	27.269	19.579	1.00
	ATOM 18.85	1535 A		PRO	A	209	-	0.088	28.644	19.701	1.00
20	ATOM 17.85			PRO	A	209		0.477	29.457	18.545	1.00
	ATOM 17.50	1537 A		PRO	A	209	-	0.483	26.483	17.368	1.00
		1538 A	0	PRO	A	209	-	1.094	27.157	16.558	1.00
25	ATOM 16.70	1539 A	Ń N	THR	A	210	-	0.816	25.240	17.652	1.00
	ATOM 17.34	1540 A	CA C	THR	Α	210		2.050	24.690	17.186	1.00
30	ATOM 16.73	1541 A	CB C	THR	A	210	-	2.042	23.181	17.356	1.00
	ATOM 18.34	1542 A	OG1 O		A	210		1.848	22.859	18.734	1.00

	ATOM 16.90	1543 A		THR	A	210	-0.833	22.540	16.574	1.00
		1544 A		THR	A	210	-3.206	25.327	17.987	1.00
5		1545 A		THR	Α	210	-2.990	26.095	18.930	1.00
		1546 A		ARG	A	211	-4.421	24.979	17.623	1.00
10				ARG	A	211	-5.595	25.577	18.264	1.00
	ATOM 21.16			ARG	A	211	-6.884	25.056	17.638	1.00
	ATOM 25.92	1549 A		ARG	A	211	-8.149	25.719	18.255	1.00
15	ATOM 31.08	1550 A		ARG	A	211	-9.325	25.804	17.301	1.00
		1551 A		ARG	A	211	-8.956	26.457	16.042	
20	ATOM 38.91	1552 A		ARG	A	211	-9.626	26.296	14.905	1.00
		1553 A		ARG	Α	211	-10.707	25.516	14.876	1.00
	ATOM 37.74	1554 A	NH2 N	ARG	Α	211	-9.225	26.911	13.795	1.00
25	ATOM 20.16	1555 A	C C	ARG	Α	211	-5.591	25.308	19.768	1.00
	ATOM 19.93	1556 A	0 0	ARG	A	211	-5.983	26.180	20.539	1.00
30	ATOM 19.40	1557 A	N N	ASP	Α	212	-5.120	24.121	20.185	1.00
	ATOM 18.64	1558 A	CA C	ASP	Α	212	-5.031	23.791	21.616	1.00

	ATOM 18.58	1559 A		ASP	A	212	-5.346	22.306	21.877	1.00
	ATOM 16.59	1560 A		ASP	A	212	-4.318	21.356	21.254	1.00
5	ATOM 16.40	1561 A	OD1 O	ASP	Α	212	-4.255	20.180	21.679	1.00
	ATOM 17.56	1562 A	OD2 O	ASP	Α	212	-3.545	21.688	20.339	1.00
10	ATOM 18.83	1563 A	C C	ASP	A	212	-3.693	24.160	22.255	1.00
	ATOM 19.22			ASP	A	212	-3.387	23.707	23.370	1.00
	ATOM 18.29	1565 A	N N	GLY	A	213	-2.902	24.966	21.556	1.00
15	ATOM 18.10	1566 A		GLY	A	213	-1.698	25.572	22.111	1.00
	ATOM 17.75		C C	GLY	A	213	-0.439	24.713	22.065	1.00
20	ATOM 18.06	1568 A		GLY	A	213	0.517	24.998	22.785	1.00
	ATOM 16.43		N N	ARG	A	214	-0.431	23.665	21.242	1.00
	ATOM 16.72	1570 A	CA C	ARG	A	214	0.757	22.826	21.110	1.00
25	ATOM 16.17	1571 A		ARG	A	214	0.403	21.461	20.536	1.00
	ATOM 16.40	1572 A	CG C	ARG	A	214	-0.276	20.553	21.473	1.00
30	ATOM 16.61	1573 A		ARG	A	214	-0.753	19.301	20.814	1.00
	ATOM 16.67	1574 A		ARG	A	214	-1.771	19.613	19.826	1.00

	ATOM 16.71	1575 A	CZ C		A	214	-1.740	19.297	18.531	1.00
	ATOM 16.55	1576 A	NH1 N		A	214	-0.720	18.628	17.981	1.00
5	ATOM 14.42		NH2 N		A	214	 -2.762	19.664	17.776	1.00
	ATOM 16.16	1578 A	C C	ARG	A	214	1.772	23.493	20.203	
10	ATOM 16.86	1579 A	0	ARG	A	214	1.403	24.306	19.344	1.00
	ATOM 15.82	1580 A		ILE	A	215	3.046	23.168	20.396	1.00
	ATOM 15.40	1581 A		ILE	A	215	4.107	23.640	19.516	
15	ATOM 16.18	1582 A		ILE	Α	215	5.503	23.498	20.175	1.00
	ATOM 17.35	1583 A	CG1 C	ILE	A	215	5.600	24.351	21.454	1.00
20	ATOM 20.01	1584 A		ILE	A	215	5.526	25.842	21.181	1.00
	ATOM 15.87	1585 A		ILE	A	215	6.606	23.898	19.191	1.00
	ATOM 15.40	1586 A		ILE	A	215	4.100	22.834	18.214	1.00
25		1587 A		ILE	A	215	4.316	21.616	18.227	1.00
	ATOM 14.61	1588 A	N N	LYS	Α	216	3.841	23.536	17.117	1.00
30	ATOM 14.64	1589 A	CA C	LYS	A	216	4.072	23.062	15.745	1.00
	ATOM 13.98	1590 A	CB C	LYS	A	216	2.765	22.616	15.067	,1.00

	ATOM 13.46	1591 A		LYS	A	216	2.190	21.271	15.526	1.00
	ATOM 14.36	1592 A		LYS	A	216	3.073	20.102	15.117	1.00
5	ATOM 13.24	1593 A		LYS	A	216	2.427	18.754	15.453	1.00
	ATOM 8.08	1594 A		LYS	A	216	3.042	17.577	14.739	1.00
10	ATOM 14.70			LYS	A	216	4.632	24.269	14.984	1.00
	ATOM 13.92	1596 A		LYS	A	216	4.336	25.428	15.358	1.00
	ATOM 14.59		N N	PRO	Α	217	5.410	24.032	13.921	1.00
15	ATOM 13.65	1598 A		PRO	Α	217	5.788	22.691	13.468	1.00
	ATOM 14.58			PRO	A	217	6.452	22.944	12.115	1.00
20	ATOM 15.23	1600 A		PRO	Α	217	6.934	24.356	12.178	1.00
	ATOM 14.44	1601 A		PRO	A	217	6.012	25.077	13.086	1.00
	ATOM 12.99	1602 A		PRO	Α	217	6.818	22.089	14.401	1.00
25	ATOM 12.11			PRO	A	217	7.262	22.738	15.379	1.00
	ATOM 11.74	1604 A		ASP	A	218	7.201	20.847	14.126	1.00
30		1605 A		ASP	Α	218	8.188	20.214	14.974	1.00
	ATOM 11.47			ASP	Α	218	8.033	18.694	14.962	1.00

	ATOM 11.82	1607 A	CG C	ASP	A	218	6.67	2 18.24	1 15.451	1.00
	ATOM 10.57	1608 A	OD1 O	ASP	Α	218	6.44	0 18.37	0 16.680	1.00
5	ATOM 11.50	1609 A	OD2 O	ASP	Α	218	5.81	0 17.72	6 14.671	1.00
	ATOM 11.30	1610 A	C C	ASP	A	218	9.61	9 20.56	6 14.610	1.00
10	ATOM 10.85	1611 A	0	ASP	A	218	10.44	1 20.77	2 15.501	1.00
	ATOM 11.61	1612 A	N N	VAL	A	219	9.92	8 20.51	6 13.314	1.00
	ATOM 12.37	1613 A	CA C	VAL	A	219	11.25	4 20.82	9 12.815	1.00
15	ATOM 12.19	1614 A	CB C	VAL	A	219	12.11	8 19.58	9 12.602	1.00
	ATOM 14.24	1615 A	CG1 C	VAL	A	219	12.40	1 18.86	7 13.933	1.00
20	ATOM 13.54	1616 A		VAL	A	219	11.48	5 18.66	0 11.587	1.00
	ATOM 12.33		C C	VAL	A	219	11.14	8 21.56	8 11.471	1.00
	ATOM 12.34		0 0	VAL	Α	219	10.08	3 21.62	4 10.851	1.00
25	ATOM 11.78	1619 A	N N	MET	A	220	12.26	6 22.13	9 11.057	1.00
	ATOM 11.89	1620 A	CA C	MET	A	220	12.36	5 22.930	9.852	1.00
30	ATOM 11.30	1621 A	CB C	MET	A	220	12.79	8 24.37	1 10.167	1.00
	ATOM 11.64	1622 A		MET	A	220	12.02	5 25.05	8 11.255	1.00

	ATOM 12.02	1623 A		MET	Α	220	10.310	25.322	10.860	1.00
	ATOM 11.35	1624 A		MET	A	220	10.416	26.727	9.791	1.00
5	ATOM 12.21	1625 A		MET	A	220	13.398	22.343	8.902	1.00
	ATOM 12.24	1626 A		MET	A	220	14.368	21.731	9.321	1.00
10	ATOM 12.60	1627 A			A	221	13.175	22.556	7.613	1.00
	ATOM 12.90	1628 A		ALA	A	221	14.198	22.324	6.605	1.00
	ATOM 12.23	1629 A	CB C	ALA	Α	221	14.098	20.912	6.081	1.00
15	ATOM 13.77	1630 A		ALA	A	221	14.064	23.341	5.464	1.00
	ATOM 14.46	1631 A		ALA	A	221	13.029	24.027	5.312	1.00
20	ATOM 13.99	1632 A	N N	PRO	A	222	15.116	23.487	4.687	1.00
	ATOM 14.73	1633 A	CA C	PRO	A	222	15.059	24.393	3.543	1.00
	ATOM 13.69	1634 A	CB C	PRO	A	222	16.387	24.159	2.845	1.00
25	ATOM 15.06			PRO	Α	222	17.290	23.676	3.892	1.00
	ATOM 14.39	1636 A		PRO	Α	222	16.433	22.855	4.830	1.00
30	ATOM 14.82	1637 A		PRO	Α	222	13.896	24.044	2.622	1.00
	ATOM 15.21	1638 A		PRO	A	222	13.719	22.847	2.284	1.00

	ATOM 14.57	1639 A			A 223	13.178	25.069	2.193	1.00
	ATOM 15.06	1640 A			A 223	11.996	24.910	1.373	1.00
5	ATOM 14.81	1641 A			A 223	11.779	26.046	0.383	1.00
	ATOM 15.67	1642 A			A 223	10.661	26.268	-0.039	1.00
10	ATOM 13.98	1643 A			A 224	12.822	26.799	0.049	1.00
	ATOM 14.01	1644 A		THR A	A 224	12.706	27.772	-1.007	1.00
	ATOM 13.98	1645 A			A 224	12.912	29.229	-0.517	1.00
15	ATOM 13.39	1646 · A	OG1 O	THR A	. 224	14.220	29.350	0.047	1.00
	ATOM 14.59	1647 A	CG2 C	THR A	224	11.952	29.585	0.597	1.00
20	ATOM 14.02			THR A	A 224	13.729	27.449	-2.072	1.00
	ATOM 14.13	1649 A		THR A	224	14.813	26.932	-1.791	1.00
	ATOM 14.73		N N	TYR A	225	13.389	27.786	-3.308	1.00
25	ATOM 14.78	1651 A		TYR A	225	14.270	27.528	-4.441	1.00
	ATOM 15.26	1652 A	CB C	TYR A	225	15.197	28.726	-4.686	1.00
30	ATOM 15.90	1653 A		TYR A	225	14.502	29.848	-5.398	1.00
	ATOM 18.12	1654 A	CD1 C	TYR A	225	14.027	30.940	-4.692	1.00

	ATOM 18.57	1655 A		TYR	Α	225	13.349	31.960	-5.301	1.00
	ATOM 19.46	1656 A		TYR	A	225	13.100	31.918	-6.659	1.00
5	ATOM 20.70	1657 A	OH O	TYR	A	225	12.391	32.974	-7.207	1.00
	ATOM 18.30	1658 A		TYR	A	225	13.510	30.844	-7.404	1.00
10	ATOM 19.15	1659 A	CD2 C	TYR	A	225	14.225	29.788	-6.771	1.00
	ATOM 14.79	1660 A	C C	TYR	A	225	15.022	26.196	-4.331	1.00
	ATOM 15.52	1661 A	0	TYR	A	225	16.252	26.119	-4.395	1.00
15	ATOM 15.07	1662 A	N N	ILE	A	226	14.248	25.130	-4.186	1.00
	ATOM 14.45	1663 A	CA C	ILE	A	226	14.773	23.759	-4.155	1.00
20	ATOM 14.35	1664 A	CB C	ILE	Α	226	13.904	22.866	-3.254	1.00
	ATOM 15.47	1665 A	CG1 C	ILE	A	226	13.906	23.341	-1.789	1.00
	ATOM 16.51	1666 A	CD1 C	ILE	A	226	15.239	23.250	-1.085	1.00
25	ATOM 14.04			ILE	Α	226	14.312	21.400	-3.377	1.00
	ATOM 14.24			ILE	A	226	14.780	23.205	-5.580	1.00
30	ATOM 13.78	1669 A		ILE	A	226	13.778	23.188	-6.245	1.00
	ATOM 14.94	1670 A			Α	227	15.937	22.753	-6.022	1.00

	ATOM 14.97	1671 A			A	227		16.141	22.230	-7.359 ·	1.00
	ATOM 15.61	1672 A	CB C	LEU	A	227		17.541	22.653	-7.827	1.00
5	ATOM 16.60	1673 A		LEU	A	227		17.950	22.137	-9.196	1.00
	ATOM 16.90	1674 A		LEU.	A	227		16.899	22.508	-10.231	1.00
10	ATOM 18.98	1675 A	CD2 C	LEU	A	227		19.340	22.669	-9.559	1.00
	ATOM 14.76	1676 A		LEU	A	227		16.010	20.708	-7.284	1.00
	ATOM 15.34			LEU	A	227		16.803	20.038	-6.602	1.00
15	ATOM 14.03		N N	SER	Α	228		14.970	20.179	-7.924	1.00
	ATOM 14.07	1679 A	CA C	SER	A	228		14.665	18.752	-7.871	1.00
20	ATOM 13.81	1680 . A		SER	Α	228		13.701	18.448	-6.701	1.00
	ATOM 12.38	1681 A		SER	A	228		13.631	17.038	-6.453	1.00
	ATOM 14.98	1682 A	C C	SER	A	228		14.061	18.319	-9.208	1.00
25	ATOM 15.43	1683 A	0	SER	A	228		13.971	19.115	-10.133	1.00
	ATOM 14.57	1684 A	N N	ALA	A	229		13.626	17.067	-9.278	1.00
30	ATOM 14.87	1685 A	CA C	ALA	A	229		13.155	16.454	-10.516	1.00
	ATOM 14.78	1686 A	CB C	ALA	A	229	-	12.824	14.945	-10.268	1.00

	ATOM 14.83	1687 A	C C	ALA	Α	229	11.9	39 1	L7.135	-11.086	1.00
	ATOM 14.22	1688 A	0	ALA	A	229	10.9	39 1	17.411	-10.376	1.00
5	ATOM 14.42	1689 A	N N	ARG	Α	230	12.0	27 1	17.381	-12.394	1.00
	ATOM 14.49	1690 A	CA C	ARG .	A	230	10.9	74 1	8.013	-13.155	1.00
10	ATOM 14.60	1691 A	CB C	ARG .	A	230	11.5	53 1	9.008	-14.137	1.00
	ATOM 16.55	1692 A	CG C	ARG 2	A	230	10.5	16 1	9.626	-15.065	1.00
	ATOM 19.98	1693 A	CD C	ARG Z	A	230	11.0	44 2	0.792	-15 <sup>-</sup> .934	1.00
15	ATOM 19.63	1694 A	NE N	ARG A	A	230	9.9	40 2	1.308	-16.751	1.00
	ATOM 21.34	1695 A	CZ C	ARG A	Ą	230	9.6	92 2	2.581	-16.995	1.00
. 20	ATOM 21.55	1696 A	NH1 N	ARG A	Ā	230	10.5	02 2	3.547	-16.545	1.00
	ATOM 20.71	1697 A	NH2 N	ARG A	Ā	230	8.6	17 2	2.898	-17.730	1.00
	ATOM 14.81	1698 A	Ċ C	ARG A	Ą	230	10.2	32 1	6.947	-13.948	1.00
25	ATOM 14.40	1699 A	0 0	ARG A	A	230	10.8	38 1	6.237	-14.762	1.00
	ATOM 14.68	1700 A	N N	SER A	Ą	231	8.9	31 1	6.837	-13.703	1.00
30	ATOM 15.32	1701 A	CA C	SER A	Δ.	231	8.10	06 1	5.937	-14.463	1.00
	ATOM 15.75	1702 A	CB C	SER A	<b>.</b> .	231	6.66	50 1	6.034	-14.030	1.00

	ATOM 16.08	1703 A	OG O		A	231	5.836	15.317	-14.947	1.00
	ATOM 15.44	1704 A	C		A	231	8.176	16.325	-15.956	1.00
5	ATOM 13.31	1705 A	0		A	231	8.087	17.494	-16.306	1.00
	ATOM 15.69	1706 A	N N		A	232	8.295	15.321	-16.802	1.00
10	ATOM 16.52	1707 A	CA C	SER	A	232	8.323	15.494	-18.255	1.00
	ATOM 16.29	1708 A	CB C	SER	Α	232	8.682	14.156	-18.906	1.00
	ATOM 16.72	1709 A	OG O	SER	A	232	7.610	13.191	-18.730	1.00
15	ATOM 18.10	1710 A	C C	SER	A	232	7.004	16.050	-18.820	1.00
	ATOM 18.08	1711 A	0	SER	A	232	6.970	16.540	-19.945	1.00
20	ATOM 18.99	1712 A	N N	LEU	A	233	5.924	16.005	-18.040	1.00
	ATOM 19.87	1713 A	CA C	LEU	A	233	4.647	16.550	-18.466	1.00
	ATOM 20.52	1714 A		LEU	Α	233	3.503	15.655	-17.989	1.00
25	ATOM 22.45	1715 A		LEU	A	233	3.579	14.202	-18.428	1.00
	ATOM 25.84	1716 A		LEU	A	233	2.344	13.472	-17.943	1.00
30	ATOM 26.24	1717 A		LEU	A	233	3.683	14.146	-19.948	1.00
	ATOM 20.22		C C	LEU	Α	233	4.357	17.956	-17.940	1.00

	ATOM 20.30	1719 A	0	LEU	A	233	3.365	18.546	-18.345	1.00
	ATOM 18.84	1720 A	N N	ALA	A	234	5.164	18.485	-17.016	1.00
5	ATOM 19.34	1721 . A	CA C	ALA	A	234	4.768	19.731	-16.365	1.00
	ATOM 18.58	1722 A	CB C	ALA	Α	234	5.297	19.781	-14.958	1.00
10	ATOM 19.93	1723 A	C C	ALA	Α	234	5.197	20.991	-17.153	1.00
	ATOM 20.41	1724 A	0	ALA	A	234	6.300	21.037	-17.701	1.00
	ATOM 20.75	1725 A	N N	PRO	Α	235	4.325	21.989	-17.197	1.00
15	ATOM 21.88	1726 A	CA C	PRO	A	235	4.642	23.288	-17.802	1.00
	ATOM 21.83	1727 A	CB C	PRO	A	235	3.271	23.921	-17.981	1.00
20	ATOM 21.93	1728 A	CG C	PRO	Α	235	2.429	23.326	-16.902	1.00
	ATOM 21.22	1729 A	CD C	PRO	Α	235	2.947	21.944	-16.677	1.00
	ATOM 22.70	1730 A		PRO	A	235	5.495	24.199	-16.885	1.00
25	ATOM 21.06	1731 A	0	PRO	Α	235	5.513	23.970	-15.671	1.00
	ATOM 24.00	1732 A	N N	ASP	Α	236	6.150	25.204	-17.489	1.00
30	ATOM 24.41	1733 A	CA C	ASP	Α	236	6.960	26.228	-16.795	1.00
	ATOM 24.21	1734 A	CB C	ASP	A	236	7.455	27.332	-17.750	1.00

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	ATOM 25.42	1735 A	ASP	A	236	8.603	26.838	-18.636	1.00
	ATOM 25.18		ASP	Α	236	9.214	27.656	-19.365	1.00
5	ATOM 23.87	1737 A	ASP	A	236	8.990	25.634	-18.674	1.00
		1738 A	ASP	A	236	6.263	26.644	-15.520	1.00
10	ATOM 24.16		ASP	A		6.919	27.035	-14.558	1.00
	ATOM 25.32		SER	A	237	4.933	26.677	-15.491	1.00
	ATOM 24.89	1741 A	SER	A	237	4.179	27.723	-14.873	1.00
15	ATOM 25.98	1742 A	SER	A	237	2.801	27.926	-15.490	1.00
	ATOM 27.95		SER	A	237	2.035	26.723	-15.436	1.00
20		1744 A	SER	A	237	4.027	26.960	-13.487	1.00
	ATOM 23.01	1745 A	SER	A	237	3.588	27.516	-12.495	1.00
	ATOM 22.59	1746 A	SER	A	238	4.363	25.660	-13.448	1.00
25		1747 A	SER	Α	238	4.313	24.861	-12.201	1.00
	ATOM 22.11	1748 A	SER	Α	238	4.238	23.344	-12.501	1.00
30	ATOM 22.38		SER	Α	238	3.046	22.968	-13.146	1.00
	ATOM 21.86	1750 A	SER	Α	238	5.543	25.045	-11.295	1.00

	ATOM 22.29	1751 A	0		Α	238		5.550	24.542	-10.184	1.00
	ATOM 21.32	1752 A	N N		Α	239		6.568	25.744	-11.789	1.00
5	ATOM 20.67	1753 A	CA C	PHE	A	239		7.847	25.899	-11.108	1.00
	ATOM 20.17	1754 A	CB C	PHE	Α	239		8.966	25.299	-11.966	1.00
10	ATOM 20.18	1755 A		PHE	Α	239		8.736	23.854	-12.294	1.00
	ATOM 18.34	1756 A		PHE	A	239		8.964	22.881	-11.344	1.00
	ATOM 15.67	1757 A	CE1 C	PHE	<b>A</b>	239		8.686	21.573	-11.600	1.00
15	ATOM 16.81	1758 A	CZ C	PHE	A	239		8.194	21.184	-12.814	1.00
	ATOM 16.81	1759 A		PHE	A	239		7.924	22.128	-13.775	1.00
20	ATOM 18.63		CD2 C	PHE	A	239		8.194	23.466	-13.520	1.00
	ATOM 20.81	1761 A		PHE	A	239		8.124	27.370	-10.775	1.00
		1762 A		PHE	A	239		7.589	28.283	-11.404	1.00
25		1763 A		TRP	A	240		8.927	27.575	-9.743	1.00
		1764 A		TRP	A	240		9.420	28.913	-9.382	1.00
30	ATOM 21.05	1765 A		TRP	A	240		10.192	28.842	-8.055	1.00
		1766 A		TRP	A	240	-	9.324	28.850	-6.857	1.00

	ATOM 23.97	1767 A		TRP	A	240	8.027	28.446	-6.782	1.00
	ATOM 24.62	1768 A		TRP	A	240	7.548	28.624	-5.509	1.00
5	ATOM 24.31	1769 A		TRP	A	240	8.547	29.148	-4.726	1.00
	ATOM 23.24	1770 A	CD2 C	TRP	Α	240	9.677	29.302	-5.537	1.00
10	ATOM 24.95	1771 A	CE3 C	TRP	A	240	10.839	29.811	-4.966	1.00
	ATOM 24.14	1772 A		TRP	A	240	10.833	30.146	-3.637	1.00
	ATOM 23.89	1773 A	CH2 C	TRP	A	240	9.682	29.991	-2.857	1.00
15	ATOM 25.05	1774 A	CZ2 C	TRP	A	240	8.542	29.483	-3.378	1.00
	ATOM 20.95	1775 A	C C	TRP	A	240	10.355	29.466	-10.461	1.00
20	ATOM 20.42	1776 A		TRP	A	240	10.419	30.673	-10.703	1.00
	ATOM 21.11	A	N				11.097	28.566	-11.080	1.00
	21.52	1778 A	С						-12.149	
25	ATOM 21.93	A	С				13.243			
	ATOM 21.79	1780 A	С				12.466			ſ
30	ATOM 22.05	1781 A	0							1.00
	ATOM 22.09	1782 A	N N	ASN	A	242	12.929	27.769	-14.040	1.00

	ATOM 22.74	1783 A		ASN	A	242		13.481	26.656	-14.800	1.00
	ATOM 22.69	1784 . A		ASN	A	242		13.397	26.962	-16.322	1.00
5	ATOM 22.96	1785 A		ASN	A	242		11.960	27.071	-16.828	1.00
	ATOM 21.33	1786 A	OD1 O	ASN	A	242		11.024	26.578	-16.198	1.00
10	ATOM 21.31	1787 A	ND2 N	ASN	Α	242	ě	11.782	^27.727	-17.969	1.00
	ATOM 23.18	1788 A	C C	ASN	Α	242	·	14.927	26.359	-14.458	1.00
	ATOM 23.35	1789 A	0	ASN	A	242		15.634	27.194	-13.902	1.00
15	ATOM 24.21	1790 A	N N	HIS	A	243		15.375	25.169	-14.820	1.00
	ATOM 25.06	1791.^ A		HIS	A	243		16.802	24.875	-14.862	1.00
20	ATOM 25.31	1792 A	CB · C	HIS	A	243		17.234	24.062	-13.653	1.00
	ATOM 27.16		CG C	HIS	A	243	. <del>-</del>	18.703	23.809	-13.595	1.00
	ATOM 30.11			HIS	Α	243		19.599	24.733	-13.086	1.00
25	ATOM .	1795 A	CE1 C	HIS	Α	243		20.820	24.231	-13.152	1.00
		1796 A	NE2 ·N	HIS	A	243		20.752	23.036	-13.713	1.00
	ATOM 28.73	1797 A	CD2 C	HIS	Α	243		19.442	22.754	-14.008	1.00
-	ATOM 26.02			HIS	A	243	•	17.158	24.144	-16.162	1.00

-	ATOM 25.77	1799 A			A	243	17.851	24.726	-17.003	1.00
	ATOM 26.20	1800 A	N N		A	244	16.711	22.880	-16.299	1.00
5	ATOM 27.35	1801 A	CA C	ASP	A	244	16.757	22.137	-17.584	1.00
	ATOM 28.02	1802 A	CB C	ASP	A	244	17.972	21.252	-17.646	1.00
10	ATOM 29.28	1803 A	CG C	ASP	A	244	18.211	20.272	-16.546	1.00
	ATOM 34.73	1804 A	OD1 O	ASP	A	244	19.393	20.188	-16.099	1.00
	ATOM 28.43	1805 A	OD2 O	ASP	A	244	17.310	19.568	-16.056	1.00
15	ATOM 27.57	1806 A	C C	ASP	A	244	15.427	21.429	-17.760	1.00
	ATOM 27.11	1807 A	0	ASP	A	244	14.751	21.208	-16.721	1.00
20	ATOM 27.83	1808 A	N N	SER	A	245	15.290	20.734	-18.836	1.00
	ATOM 26.73	1809 A	CA C	SER	A	245	14.559	19.557	-19.209	1.00
	ATOM 26.99	1810 A		SER	A	245	15.083	18.972	-20.483	1.00
25	ATOM 27.12		OG O	SER	A	245	15.792	17.785	-20.481	1.00
	ATOM 25.28	1812 A	C C	SER	A	245	14.234	18.594	-18.102	1.00
30	ATOM 24.66	1813 A		SER	A	245	13.146	17.973	-18.152	1.00
	ATOM 23.51	1814 A	N N	LYS	A	246	15.122	18.339	-17.176	1.00

	ATOM 22.90	1815 A			ВА	. 246	14.918	17.304	-16.177	1.00
	ATOM 23.64	1816 A			Α	246	15.977	16.205	-16.332	1.00
5	ATOM 26.42	1817 A	CG C		A	246	15.852	15.384	-17.600	1.00
	ATOM 29.39	1818 A			A	246	17.094	14.548	-17.859	1.00
10	ATOM 32.94	1819 A	CE C		A	246	16.880	13.584	-19.018	1.00
	ATOM 37.30	1820 A	NZ N		A	246	18.070	13.501	-19.908	1.00
	ATOM 21.77	1821 A	C C	LÝS	A	246	14.812	17.762	-14.740	1.00
15	ATOM 19.24	1822 A	0	LYS	A	246	14.396	17.059	-13.828	1.00
	ATOM 20.43	1823 A	N N	TYR	A	247	15.126	19.026	-14.452	1.00
20	ATOM 19.83	1824 A	CA C	TYR	Α	247	15.144	19.544	-13.079	1.00
	ATOM 19.35	1825 A	CB C	TYR	A	247	16.541	19.398	-12.456	1.00
	ATOM 19.14	1826 A		TYR	A	247	17.007	17.966	-12.434	1.00
25	ATOM 21.08	1827 A		TYR	A	247	17.784	17.442	-13.482	1.00
	ATOM 17.97	1828 A		TYR	A	247	18.170	16.121	-13.489	1.00
30	ATOM 19.97	1829 A	CZ. C	TYR	Α	247	17.780	15.292	-12.458	1.00
	ATOM 18.06	1830 A	ОН	TYR	Α	247	18.159	13.964	-12.465	1.00

	ATOM 18.19	1831 A		TYR	Α	247	16.999	15.781	-11.417	1.00
	ATOM 19.09	1832 A		TYR	A	247	16.630	17.109	-11.408	1.00
5	ATOM 18.89			TYR	A	247	14.697	21.003	-13.069	1.00
		1834 A		TYR	A	247	15.017	21.761	-13.994	1.00
10	ATOM 17.07	1835 A		ALA	A	248	13.936	21.385	-12.046	1.00
		1836 A		ALA	A	248	13.512	22.769	-11.893	1.00
	ATOM 15.85	1837 A				248	12,294	23.035	-12.733	1.00
15		1838 A		ALA	A	248	13.253	23.110	-10,425	1.00
	ATOM 15.81	1839 A		ALA	A	248	13.358	22.236	-9.549	1.00
20	ATOM 15.33			TYR	A	249	12.956	24.384	-10.174	1.00
	ATOM 15.08	1841 A		TYR	A	249	12.910	24.949	-8.832	1.00
		1842 A		TYR	Α	249	13.520	26.336	-8.802	1.00
25	ATOM 15.33	1843 A		TYR	A	249	14.999	26.398	-9.087	1.00
	ATOM 17.29	1844 A		TYR	A	249	15.470	26.675	-10.370	1.00
30	ATOM 16.19			TYR	Α	249	16.829	26.754	-10.640	1.00
	ATOM 18.72		CZ C	TYR	A	249	17.741	26.557	-9.608	1.00

	ATOM 21.92	1847 A			A	249		19.088	26.649	-9.839	1.00
	ATOM 18.20	1848 A			Α	249		17.306	26.287	-8.330	1.00
5	ATOM 17.03	1849 A			Α	249		15.930	26.207	-8.070	1.00
	ATOM 15.50	1850 A		TYR	Α	249		11.497	25.078	-8.358	1.00
10	ATOM 16.06	1851 A			Α	249		10.599	25.480	-9.122	1.00
	ATOM 15.10	1852 A			A	250		11.291	24.749	-7.082	1.00
	ATOM 15.40	1853 A		MET	A	250	-	10.015	24.967	-6.430	1.00
15	ATOM 15.90	1854 A		MET	Α	250		9.153	23.703	-6.542	1.00
	ATOM 19.64	1855 A	CG C	MET	A	250		7.677	23.947	-6.729	1.00
20	ATOM 23.44	1856 A	SD S	MET	A	250		6.677	22.370	-6.869	1.00
	ATOM 22.96	1857 A	CE C	MET	A	250		7.321	21.709	-8.163	1.00
	ATOM 15.09	1858 A	C C	MET	Α	250		10.274	25.318	-4.966	1.00
25	ATOM 15.78	1859 A	0 0		A	250		11.366	25.081	-4.440	1.00
	ATOM 14.69	1860 A	N N	GLY .	A	251		9.279	25.888	-4.314	1.00
30	ATOM 13.76	1861 A	CA C	GLY A	<b>A</b> :	251		9.373	26.203	-2.902	1.00
	ATOM 14.49	1862 A	C C	GLY 2	A :	251		8.026	26.058	-2.248	1.00

	ATOM 13.60	1863 A		GLY	A	251	6.984	26.057	-2.933	1:00
	ATOM 12.84				·A	252	8.056	25.926	-0.920	1.00
5	ATOM 13.22	1865 A		GLY	A	252	6.879	25.694	-0.101	1.00
	ATOM 12.42			GLY	A	252	7.242	24.765	1.058	1.00
10	ATOM 11.46			GLY	A	252	8.354	24.185	1.073	1.00
	ATOM 12.37				A	253	6.328	24.598	2.008	1.00
	ATOM 12.51	1869 A		THR	A	253	6.518	23.583	3.043	1.00
15	ATOM 13.05	1870 A		THR	Α	253	5.543	23.697	4.256	1.00
	ATOM 11.78			THR	<b>A</b>	253	4.138	23.788	3.858	1.00
20	ATOM 13.23			THR	Α	253	5.837	24.964	5.042	1.00
	ATOM 12.60	1873 A		THR	A	253	6.463	22.211	2.396	1.00
	ATOM 12.54	1874 A	0 0	THR	A	253	6.945	21.239	2.966	1.00
25	ATOM 12.69			SER	A	254	5.902	22.158	1.187	1.00
	ATOM 12.54	1876 A		SER	A	254	5.905	20.957	0.357	1.00
30	ATOM 12.41	1877 A	CB C	SER	A	254	5.228	21.233	-0.994	1.00
	ATOM 11.90	1878 A		SER	A	254	3.822	21.002	-0.960	1.00

	ATOM 12.52	1879 A			A	254		7.298	20.445	0.050	1.00
	ATOM 12.45	1880 A			A	254		7.459	19.253	-0.150	1.00
5	ATOM 12.52				Α	255		8.255	21.361	-0.054	1.00
	ATOM 13.23	1882 A			A	255		9.640	21.062	-0.385	1.00
10	ATOM 13.16	1883 A		MET	A	255		10.260	22.231	-1.164	1.00
	ATOM 13.61	1884 A			A	255		9.955	22.255	-2.667	1.00
		1885 A		MET	A	255		8.220	22.693	-3.027	1.00
15	ATOM 13.35	1886 A		MET	A	255		7.683	21.071	-3.591	1.00
	ATOM 13.32	1887 A		MET	A	255		10.478	20.759	0.873	1.00
20	ATOM 13.21	1888 A		MET	A	255		11.396	19.934	0.847	1.00
	ATOM 12.98	1889 A		ALA	Α	256	<i>)</i> .	10.162	21.415	1.981	1.00
	ATOM 12.47	1890 A		ALA	A	256		10.904	21.161	3.213	1.00
25	ATOM 11.99		CB C	ALA	A	256		10.516	22.175	4.265	1.00
	ATOM 11.89	1892 A	C C	ALA	A	256		10.645	19.737	3.717	1.00
30	ATOM 11.48	1893 A		ALA	A	256		11.553	19.018	4.179	1.00
	ATOM 11.55	1894 A	N N	THR	A	257		9.390	19.341	3.629	1.00

	ATOM 11.50	1895 A		THR	A	257	8.944	18.065	4.146	1.00
		1896 A		THR	A	257	7.423	17.938	3.908	1.00
5	ATOM 13.08			THR	A	257	6.754	19.013	4.569	1.00
	ATOM 12.46			THR	Α	257	6.838	16.661	4.540	1.00
10	ATCM 11.20			THR	Α	257	9.705	16.849	3.587	1.00
	ATOM 11.03			THR	A	257	10.172	16.018	4.382	1.00
	ATOM 11.22			PRO	Α	258	9.781	16.686	2.259	1.00
15		1902 A		PRO	A	258	10.466	15.521	1.687	1.00
	ATOM 10.45			PRO	A	258	10.200	15.644	0.182	1.00
20	ATOM 11.62			PRO	A	258	9.884	17.057	-0.029	1.00
	ATOM 10.92			PRO	A	258	9.164	17.504	1.207	1.00
	ATOM 10.83			PRO	A	258	11.969	15.503	1.976	1.00
25	ATOM 9.95				A	258	12.524	14.417	2.020	1.00
	ATOM 11.19		N N		A	259	12.605	16.665	2.160	1.00
30	ATOM 11.51			ILE	Α	259	14.004	16.711	2.597	1.00
	ATOM 11.81	1910 A		ILE	A	259	14.439	18.183	2,712	1.00

		1911 A		ILE	Α	259		14.492	18.843	1.314	1.00
		1912 A		ILE	Α	259		15.690	18.403	0.504	1.00
5		1913 A		ILE	A	259		15.790	18.313	3.375	1.00
		1914 A		ILE	Α	259		14.147	15.975	3.950	1.00
10	ATOM 11.81			ILE	A	259		15.038	15.133	4.124	1.00
		1916 A		VAL	A	260		13.259	16.295	4.886	1.00
	ATOM 12.26	1917 A		VAL	A	260		13.244	15.668	6.199	1.00
15	ATOM 12.30	1918 A		VAL	A	260	-	12.301	16.412	7.150	1.00
	ATOM 12.78			VAL	Α	260		12.286	15.743	8.557	1.00
20		1920 A		VAL	Α	260		12.721	17.855	7.268	1.00
	ATOM 12.24			VAL	À	260		12.847	14.185	6.106	1.00
	ATOM 12.79			VAL	A	260		13.412	13.339	6.786	1.00
25	ATOM 12.41	1923 A	N N	ALA	A	261		11.922	13.864	5.217	1.00
	ATOM 11.93	1924 A	CA C	ALA	Α	261		11.530	12.480	4.997	1.00
30	ATOM 12.16	1925 A	CB C	ALA	A	261		10.426	12.376	3.920	1.00
	ATOM 11.91	1926 Ą		ALA	A	261		12.750	11.661	4.585	1.00

	ATOM 11.34	1927 A		ALA	A	261	12.943	10.560	5.055	1.00
	ATOM 12.22	1928 A		GLY	A	262	13.550	12.186	3.665	1.00
5	ATOM 12.29	1929 A		GLY	A	262	14.794	11.533	3.291	1.00
		1930 A		GLY	A	262	15.786	11.431	4.447	1.00
10	ATOM 11.90			GLY	Α	262	16.414	10.386	4.660	1.00
	ATOM 12.20	1932 A		ASN	A	263	15.901	12.490	5.243	1.00
		1933 A		ASN	Α	263	16.744	12.433	6.435	1.00
15	ATOM 12.31	1934 A		ASN	A	263	16.772	13.773	7.170	1.00
	ATOM 13.12			ASN	Α	263	17.389	14.887	6.351	1.00
20	ATOM 15.95	1936 A		ASN	Α	263	18.326	14.681	5.525	1.00
	ATOM 9.15	1937 A		ASN	Α	263	16.924	16.073	6.600	1.00
	ATOM 11.83	1938 A		ASN	Α	263	16.289	11.348	7.396	1.00
25	ATOM 11.88	1 <sup>'</sup> 939 A	0 0	ASN	A	263	17.112	10.672	8.020	1.00
	ATOM 11.77	1940 A	N N	VAL	A	264	14.983	11.181	7.517	1.00
30	ATOM 12.33	1941 A	CA C	VAL	Α	264	14.425	10.138	8.367	1.00
	ATOM 12.44	1942 A	CB C	VAL	Α	264	12.893	10.268	8.506	1.00

	ATOM 12.44	1943 A	CG1 C	VAL	Α	264		.2.280	9.045	9.178	1.00
	ATOM 13.22	1944 A	CG2 C	VAL	A	264	1	12.543	11.471	9.323	1.00
5	ATOM 11.95	1945 A	C C	VAL	A	264	1	14.817	8.754	7.843	1.00
	ATOM 12.24	1946 A	O .	VAL	A	264	1	15.164	7.896	8.625	1.00
10	ATOM 12.03	1947 A	N N	ALA	A	265	1	14.813	8.553	6.527	1.00
	ATOM 11.47	1948 A	CA C	ALA	Α	265	1	.5.279	7.292	5.966	1.00
	ATOM 11.96	1949 A	CB C	ALA	A	265	1	.5.018	7.237	4.460	1.00
15	ATOM 11.77	1950 A	C C	ALA	A	265	1	6.746	7.046	6.293	1.00
	ATOM 11.77	1951 A	0 0	ALA	A	265	1	7.139	5.932	6.592	1.00
20	ATOM 12.48	1952 A	N N	GLN	A	266	1	7.571	8.091	6.262	1.00
	ATOM 11.99	1953 A	CA C	GLN	Α	266	1	.8.999	7.940	6.586	1.00
	ATOM 10.90	1954	CB C	GLN	Α	266	1	.9.782	9.230	6.311	1.00
25			CG C	GLN	Α	266	1	9.786	9.691	4.865	1.00
	ATOM 12.24		_	GLN	Α	266	2	20.548	11.011	4.671	1.00
30	ATOM			GLN	A	266	2	1.762	11.028	4.352	1.00
50	ATOM 8.53			GLN	A	266	1	.9.857	12.088	4.853	1.00

	ATOM 12.14	1959 A			A	266	19.159	7.571	8.046	1.00
	ATOM 12.13	1960 A			A	266	19.927	6.688	8.398	1.00
5	ATOM 12.44				A	267	18.463	8.305	8.898	1.00
	ATOM 12.06	1962 A			A	267	18.473	8.049	10.317	1.00
10	ATOM 12.45	1963 A	CB C		A	267	17.624	9.107	11.014	1.00
	ATOM 12.15	1964 A		LEU	A	267	17.550	9.097	12.540	1.00
	ATOM 12.99	1965 A		LEU	A	267	18.918	9.293	13.116	1.00
15	ATOM 12.84	1966 A	CD2 C	LEU	A	267	16.616	10.187	13.009	1.00
	ATOM 12.72	1967 A	C C	LEU	A	267	17.984	6.649	10.654	1.00
20	ATOM 12.91	1968 A	0	LEU	A	267	18.581	5.972	11.497	1.00
	ATOM 12.54	1969 A	N N	ARG	A	268	16.872	6.219	10.044	1.00
	ATOM 12.31	1970 A		ARG	Α	268	16.295	4.886	10.321	1.00
25	ATOM 12.21	1971 A		ARG	Α	268	14.961	4.722	9.577	1.00
	ATOM 12.56	1972 A		ARG	A	268	14.016	3.635	10.155	1.00
30	ATOM 14.20	.1973 A	CD C	ARG	A	268	12.652	3.605	9.510	1.00
	ATOM 14.70	1974 A	NE N	ARG	A	268	11.781	2.591	10.105	1.00

	ATOM 14.81	1975 A			A	268	11.837	1.306	9.829	1.00
	ATOM 14.11	1976 . A			A	268	12.697	0.829	8.942	1.00
5	ATOM 15.99	1977 A			A	268	10.993	0.483	10.432	1.00
	ATOM 12.37	1978 A			A	268	17.284	3.763	9.929	1.00
10	ATOM 11.86	1979 A	0	ARG	A	268	17.533	2.837	10.689	1.00
	ATOM 11.97	1980 A			Α	269	17.846	3.870	8.729	1.00
	ATOM 12.12			GLU	A	269	18.965	3.026	8.306	1.00
15	ATOM 11.36	1982 A		GLU	A	269	19.561	3.537	6.993	1.00
-	ATOM 12.78	1983 A		GLU	A	269	20.764	2.715	6.542	1.00
20	ATOM 15.24			GLU	Α	269	21.477	3.260	5.335	1.00
		1985 - A		GLU	A	269	21.277	4.447	5.007	1.00
	ATOM 16.25	1986 A	OE2 O	GLU	A	269	22.246	2.479	4.711	1.00
25	ATOM 12.56	1987 A	C C	GLU	A	269	20.082	2.954	9.354	1.00
	ATOM 12.26	1988 A	0 0	GLU	A	269	20.596	1.875	9.645	1.00
30	ATOM 12.79	1989 A	N N	HIS	Α	270	20.482	4.104	9.894	1.00
	ATOM 12.79	1990 A	CA C	HIS	Α	270	21.556	4.119	10.859	1.00

	ATOM 12.76	1991 A		A	270	21.918	5.531	11.289	1.00
,	ATOM 10.01	1992 A		A	270	23.160	5.583	12.120	0.50
5	ATOM 15.58	1993 A		A	270	23.195	5.601	12.063	0.50
	ATOM 7.23	1994 A		A	270	23.186	6.137	13.385	0.50
10	ATOM 20.08	1995 A	ND1AHIS N	<u>v</u>	270	23.243	5.459	13.432	0.50
	ATOM 6.26	1996 A		Α	270	24.404	6.019	13.885	0.50
	ATOM 20.34	1997 A		Α	270	24.498	5.548	13.839	0.50
15	ATOM 8.61		NE2BHIS N	Α	270	25.163	5.387	13.000	0.50
,	ATOM 20.61	1999 A		A	270	25.265	5.744	12.783	0.50
20		2000 A		A	270	24.405	5.102	11.888	0.50
	ATOM 18.53	2001 A		Α	270	24.475	5.782	11.659	0.50
	ATOM 12.75		C HIS	A	270	21.210	3.294	12.099	1.00
25	ATOM 12.88		O HIS	A	270	22.031	2.541	12.562	1.00
	ATOM 12.25		N PHE	A	271	20.009	3.468	12.666	1.00
30	ATOM 12.36	2005 A	CA PHE	A	271	19.642	2.680	13.834	1.00
	ATOM 12.01	2006 A	CB PHE	Α	271	18.274	3.114	14.370	1.00

		2007 A			A	271	18.328	4.292	15.293	1.00
	ATOM 12.44			PHE	Α	271	18.557	4.127	16.643	1.00
5		2009 A		PHE	A	271	18.601	5.229	17.500	1.00
		2010 A			A	271	18.400	6.479	17.016	1.00
10	ATOM 15.14			PHE	Α	271	18.145	6.655	15.663	1.00
•		2012 A			A	271	18.096	5.567	14.820	1.00
		2013 A		PHE	Α	271	19.620	1.178	13.492	1.00
15		2014 A		PHE	A	271	20.147	0.341	14.240	1.00
		2015 A		VAĻ	A	272	19.007	0.850	12.371	1.00
20	ATOM 13.79			VAL	A	272	18.765	-0.526	11.961	1.00
		2017 A		VAL	A	272	17.856	-0.539	10.706	1.00
	ATOM 15.25	2018 A		VAL	Α	272	17.977	-1.840	9.953	1.00
25	ATOM 13.55		CG2 C	VAL	Α	272	16.429	-0.264	11.112	1.00
	ATOM 14.17		C. C	VAL	Α	272	20.068	-1.276	11.689	1.00
30	ATOM 14.67		0 0	VAL	A	272	 20.242	-2.415	12.162	1.00
		2022 A	N N	LYS	A	273	20.992	-0.619	10.990	1.00

		2023 A		LYS	A	273	22.255	-1.217	10.606	1.00
	ATOM 14.93			LYS	Α	273	22.759	-0.664	9.267	1.00
5	ATOM 15.97	2025 A		LYS	A	273	21.893	-1.085	8.052	1.00
		2026 A		LYS	A	273	22.432	-0.488	6.729	1.00
10	ATOM 16.43			LYS	Α	273	21.735	-1.010	5.482	1.00
	ATOM 13.02	2028 A		LYS	A	273	22.131	-0.162	4.300	1.00
-		2029 A		LYS	A	273	23.366	-1.133	11.645	1.00
15		2030 A		LYS	A	273	24.172	-2.075	11.740	1.00
	ATOM 14.72	2031 A		ASN	A	274	23.402	-0.033	12.403	1.00
20	ATOM 15.62			ASN	Α	274	24.556	0.298	13.225	1.00
		2033 A		ASN	Α	274	25.197	1.649	12.786	1.00
	ATOM 17.59	2034 A	CG C	ASN	Α	274	25.555	1.662	11.290	1.00
25	ATOM 18.70	2035 A	OD1 O	ASN	A	274	25.285	2.647	10.543	1.00
	ATOM 13.05		ND2 <sub>.</sub>	ASN	Α	274	26.124	0.561	10.839	1.00
30	ATOM 15.60		C C	ASN	A	274	24.253	0.365	14.694	1.00
			0 0	ASN	A	274	25.165	0.449	15.465	1.00

	ATOM 14.80			ARG	Α	275		22.979	0.348	15.092	1.00
	ATOM 15.19			ARG	A <sup>'</sup>	275		22.670	0.517	16.505	1.00
5	ATOM 14.89			ARG	Α	275		22.046	1.883	16.723	1.00
	ATOM 17.88			ARG	Α	275		22.925	3.001	16.141	1.00
10				ARG	Α	275		22.682	4.354	16.748	1.00
	ATOM 15.44					275		23.098	4.391	18.146	1.00
	ATOM 18.17			ARG	Α	275		22.783	5.383	18.977	1.00
15	ATOM 17.27			ARG	A	275	·	22.080	6.422	18.540	1.00
	ATOM 17.72			ARG	A	275		23.191	5.356	20.239	1.00
20	ATOM 14.64			ARG	A	275		21.796	-0.573	17.088	1.00
	ATOM 15.75			ARG	Α	275		21.382	-0.456	18.212	1.00
	ATOM 14.66	2050 A	N N	GLY	Α	276		21.459	-1.577	16.283	1.00
25	ATOM 14.63	2051 A	CA C	GLY	A	276		20.880	-2.825	16.771	1.00
	ATOM 14.40	2052 A	C C	GLY	Α	276		19.403	-2.811	17.060	1.00
30	ATOM 13.52	2053 A	0 0	GLY	Α	276		18.863	-3.751	17.664	1.00
	ATOM 14.10	2054 A	N N	VAL	Α	277		18.729	-1.745	16.638	1.00

	ATOM 14.10	2055 A	-		. A	277	17.318	-1.618	16.894	1.00
	ATOM 14.71	2056 A			Α	. 277	17.021	-0.657	18.097	1.00
5	ATOM 14.49	2057 A			A	277	17.768	-1.058	19.354	1.00
	ATOM 15.67	2058 A		VAL	A	277	17.268	0.771	17.733	1.00
10	ATOM 13.79	2059 A			Α	. 277	16.547	-1.097	15.689	1.00
	ATOM 14.29	2060 A			ιA	. 277	17.082	-0.372,	14.853	1.00
	ATOM 14.21	2061 A		THR	A	278	15.273	-1.472	15.607	1.00
15	ATOM 14.50	2062 A		THR	A	278	14.325	-0.778	14.749	1.00
		2063 A		THR	Α	278	13.187	-1.700	14.301	1.00
20	ATOM 19.10	2064 A		THR	A	278	13.744	-2.825	13.607	1.00
	ATOM 17.53	2065 A		THR	A	278	12.304	-0.986	13.245	1.00
	ATOM 13.49	2066 A		THR	Α	278	13.760	0.394	15.526	1.00
25	ATOM 13.51		0 0	THR	Α	278	13.028	0.210	16.485	1.00
	ATOM 12.55	2068 A	N N	PRO	A	279	14.104	1.612	15.134	1.00
30	ATOM 11.32		CA C	PRO	A	279	13.679	2.803	15.896	1.00
	ATOM 11.71	2070 A		PRO	A	279	14.520	3.920	15.277	1.00

		2071 A		PRO	A	279	14.682	3.493	13.842	1.00
		2072 A			A	279	14.817	1.975	13.895	1.00
5	ATOM 11.90				Α	279	12.211	3.055	15.672	1.00
		2074 A			Α	279	11.786	3.053	14.516	1.00
10		2075 A			Α	280	11.438	3.212	16.743	1.00
		2076 A			Α	280	10.020	3.518	16.639	1.00
		2077 A			A	280	9.354	3.389	18.024	1.00
15		2078 A		LYS	A	280	9.324	1.993	18.573	1.00
		2079 A		LYS	A	280	8.273	1.192	17.861	1.00
20		2080 A		LYS	Α	280	8.012	-0.146	18.555	1.00
		2081 A		LYS	Α	280	6.935	-0.858	17.808	1.00
	ATOM 11.96	2082 A		LYS	Α	280	9.811	4.951	16.120	1.00
25		2083 A		LYS	A	280	10.710	5.782	16.200	1.00
	ATOM 12.23	2084 A	N N	PRO	A	281	8.666	5.233	15.512	1.00
30		2085 A		PRO	Α	281	8.370	6.608	15.073	1.00
	ATOM 12.25	2086 A		PRO	A	281	6.897	6.540	14.763	1.00

	ATOM 12.66			PRO	A	281	6.755	5.162	14.210	1.00
	ATOM 11.87			PRO	Α	281	7.592	4.300	15.126	1.00
5	ATOM 11.94				A	281	8.682	7.678	16.105	1.00
	ATOM 11.60			PRO	A	281	9.287	8.708	15.734	1.00
10	ATOM 11.91			SER	A	282	8.303	7.447	17.374	1.00
	ATOM 11.78			SER	A	282	8.579	8.404	18.442	1.00
	ATOM 11.85			SER	A	-282	8.017	7.930	19.789	1.00
15	ATOM 12.30			SER	A	282	8.503	6.639	20.117	1.00
	ATOM 11.36			SER	Α	282	10.049	8.704	18.654	1.00
20	ATOM 11.10			SER	A	282	10.402	9.835	19.014	1.00
	ATOM 11.81			LEU	A	283	10.896	7.696	18.498	1.00
	ATOM 11.66		CA C	LEU	A	283	12.332	7.889	18.642	1.00
25		2099 A	CB C	LEU	A	283	13.042	6.532	18.856	1.00
	ATOM 11.60	2100 A	CG C	LEU	A	283	14.575	6.628	18.893	1.00
30		2101 A		LEU	A	283	15.029	7.501	20.001	1.00
	ATOM 15.86	2102 A	CD2 C	LEU	Α	283	15.180	5.233	19.066	1.00

	ATOM 11.15			LEU	A	283	12.953	8.650	17.465	1.00
	ATOM 11.72			LEU	A	283	13.812	9.515	17.644	1.00
5	ATOM 11.65	2105 A		LEU	Α	284	12.575	8.305	16.244	1.00
	ATOM 10.89			LEU	Α	284	13.056	9.058	15.088	1.00
10	ATOM 10.71			LEU	Α	284	12.493	8.470	13.802	1.00
	ATOM 10.82			LEU	Α	284	13.010	7.059	13.442	1.00
	ATOM 10.74			LEU	Α	284	12.102	6.419	12.399	1.00
15	ATOM 10.79			LEU	A	284	14.425	7.107	12.953	1.00
	ATOM 10.24			LEU	Α	284	12.741	10.568	15.245	1.00
20	ATOM 9.64	2112 A		LEU	A	284	13.591	11.414	15.013	1.00
	ATOM 10.77			LYS	Α	285	11.527	10.868	15.682	1.00
	ATOM 10.81	2114 A	CA C	LYS	A	285	11.054	12.217	15.890	1.00
25	ATOM 10.59	2115 A	CB C	LYS	A	285	9.544	12.188	16.152	1.00
	ATOM 10.18	2116 A	CG C	LYS	A	285	8.909	13.531	16.527	1.00
30	ATOM 12.54		CD C	LYS	Α	285	7.372	13.380	16.583	1.00
	ATOM ,	2118 A		LYS	A	285	6.660	14.630	17.085	1.00

	ATOM 9.27		NZ N	LYS	Α	285	5.159	14.525	16.941	1.00
	ATOM 10.86	2120 A	C C	LYS	A	285	11.816	12.886	17.037	1.00
5	ATOM 11.16	2121 A	0 0	LYS	A	285	12.287	13.995	16.888	1.00
	ATOM 10.94	2122 A		ALA	A	286	11.964	12.194	18.156	1.00
10	ATOM 11.16			ALA	Α	286	12.744	12.722	19.280	1.00
	ATOM 11.37	2124 A		ALA	Α	286	12.657	11.813	20.437	1.00
	ATOM	2125 A		ALA	A	286	14.206	12.952	18.897	1.00
15				ALA	A	286	14.794	13.947	19.275	1.00
		2127	N	ALA	A	287	14.778	12.048	18.115	1.00
20	ATOM 12.13		CA	ALA	Α	287	16.175	12.206	17.679	1.00
20	MOTA	2129	СВ	ALA	Α	287	16.692	10.922	17.034	1.00
	MOTA		С	ALA	A	287	16.349	13.411	16.742	1.00
25	12.42 ATOM			ALA	Α	287	17.310	14.165	16.873	1.00
	11.82 ATOM	2132		LEU	Α	288		13.623	15.826	1.00
	12.37 ATOM		N CA	LEU	A	288	15.473	14.808	14.956	1.00
30		A	C	T:E:II	Α	288	14.357	14.775	13.917	1.00
	13.67	213 <del>4</del> A					· · · · · · · ·			

	ATOM 15.39	2135 A		LEU	A	288	14.552	13.833	12.736	1.00
	ATOM 19.44	2136 A		LEU	Α	288	13.379	14.033	11.840	1.00
5	ATOM 15.17	2137 A		LEU	A	288	15.842	14.113	11.974	1.00
	ATOM 12.69	2138 A		LEU	A	288	15.329	16.105	15.747	1.00
10	ATOM 12.69			LEU	Α	288	16.014	17.107	15.481	1.00
	ATOM 12.33	2140 A		ILE	Α	289	14.412	16.096	16.704	1.00
		2141 A		ILE	Α	289	14.195	17.261	17.546	1.00
15	ATOM 12.55	2142 A		ILE	A	289	12.920	17.084	18.397	1.00
	ATOM 11.46	2143 A		ILE .	A	289	11.688	17.178	17.488	1.00
20	ATOM 10.00	2144 A		ILE A	A	289	10.404	16.725	18.104	1.00
	ATOM 13.54			ILE 2	A	289	12.869	18.098	19.506	1.00
	ATOM 12.74	2146 A	C C	ILE	A	289	15.412	17.596	18.426	1.00
25	ATOM 13.36	2147 A	0 0	ILE	A	289	15.844	18.746	18.442	1.00
	ATOM 11.71	2148 A	N N	ALA	Α	290	15.975	16.612	19.132	1.00
30	ATOM 11.73	2149 A	CA C	ALA .	A	290	17.132	16.854	19.976	1.00
	ATOM 12.08	2150 A	CB C	ALA Z	A	290	17.529	15.593	20.698	1.00

	ATOM 11.95	2151 A			A	290	18.326	17.370	19.191	1.00
	ATOM 10.65	2152 . A			A	290	19.114	18.198	19.689	1.00
5	ATOM 11.84				A	291	18.472	16.866	17.979	1.00
		2154 A		GLY	A	291	19.633	17.207	17.171	1.00
10	ATOM 12.44			GLY	A	291	19.466	18.506	16.400	1.00
		2156 A			A	291	20.437	19.018	15.847	1.00
	ATOM 12.96	2157 A		ALA	A	292	18.249	19.056	16.378	1.00
15		2158 A		ALA	A	292	17.960	20.238	15.562	1.00
	ATOM 12.99			ALA	A	292	16.454	20.468	15.434	1.00
20	ATOM 13.45			ALA	A	292	18.655	21.499	16.075	1.00
	ATOM 13.95	2161 A		ALA	Ą	292	18.954	21.612	17.252	1.00
		2162 A	N N	ALA	A	293	18.848	22.456	15.173	1.00
25	ATOM 13.43	2163 A	CA C	ALA	A	293 <sup>°</sup>	19.567	23.694	15.450	1.00
	ATOM 13.22	2164 A	CB CB	ALA	A	293	20.508	24.012	14.284	1.00
30	ATOM 13.54	2165 A	C . C	ALA	A	293	18.611	24.866	15.637	1.00
	ATOM 13.39	2166 A	0 0	ALA	A	293	17.739	25.107	14.812	1.00

	ATOM 13.60	2167 A			P <u>7</u> 4	294		18.838	25.626	16.691	1.00
	ATOM 14.04	2168 A			À	. 294		18.167	26.895	16.899	1.00
5	ATOM 14.33	2169 A			A	294		18.590	27.428	18.270	1.00
	ATOM 14.83	2170 A	CG C	ASP	A	294		17.918	28.728	18.634	1.00
10	ATOM 11.77	2171 A			A	294		18.142	29.160	19.799	1.00
	ATOM 10.92	2172 A	OD2 O	ASP	A	294		17.144	29.360	17.861	1.00
	ATOM 13.72	2173 A	C C	ASP	A	294		18.620	27.814	15.774	1.00
15	ATOM 14.66	2174 A	0	ASP	A	294			28.075	15.636	1.00
	ATOM 14.43	2175 A	N N	VAL	A	295	i		28.304	14.956	1.00
20	ATOM 14.05	2176 A	CA C	VAL	Α	295		18.057	29.217	13.853	1.00
	ATOM 13.77	2177 A	CB C	VAL	Α	295		16.957	29.283	12.730	1.00
	ATOM 13.93	2178 A		VAL	A	295		16.670	27.907	12.184	1.00
25	ATOM 12.53	2179 A		VAL	Α	295		15.680	29.956	13.255	1.00
	ATOM 14.82	2180 A		VAL	A	295		18.352	30.622	14.346	1.00
30	ATOM 15.77	2181 A		VAL	A	295		18.707	31.497	13.558	1.00
	ATOM 14.99		N N	GLY	Α	296		18.190	30.857	15.646	1.00

	ATOM 15.10			GLY	Α	296	18.450	32.159	16.208	1.00
	ATOM 15.03			GLY	A	296	17.282	32.821	16.906	1.00
5	ATOM 15.00			GLY	A	296	17.458	33.886	17.489	1.00
	ATOM 16.05			LEU	A	297	16.114	32.180	16.887	1.00
10	ATOM 15.21			LEU	Α	297	14.903	32.728	17.501	1.00
	ATOM 14.95	2188 A		LEU	A	297	13.704	32.420	16.605	1.00
	ATOM 17.47			LEU	A	297	13.881	32.962	15.179	1.00
15	ATOM 19.73			LEU	A	297	12.718	32.507	14.330	1.00
	ATOM 18.75			LEU	Α	297	13.939	34.500	15.204	1.00
20		2192 A		LEU	A	297	14.645	32.187	18.903	1.00
	ATOM 14.95			LEU	A	297	13.782	32.682	19.636	1.00
	ATOM 15.28	2194 A	N N	GLY	A	298	15.380	31.152	19.266	1.00
25	ATOM 15.27	2195 A	CA C	GLY	Α	298	15.251	30.546	20.570	1.00
	ATOM 15.55	2196 A	C C	GLY	A	298	14.024	29.691	20.721	1.00
30	ATOM 15.07	2197 A	0	GLY	Α	298	13.173	29.572	19.817	1.00
	ATOM 15.47	2198 A	N N	PHE	Α	299	13.941	29.090	21.894	1.00

	ATOM 16.76	2199 A	PHE	A	299	12.820	28.269	22.266	1.00
		2200 A	PHE	A	299	13.279	26.818	22.539	1.00
5	ATOM 16.07	2201 A	PHE	Α	299	14.108	26.237	21.435	1.00
		2202 A	PHE	A	299	13.572	26.047	20.167	1.00
10			PHE	A	299	14.349	25.544	19.132	1.00
		2204 A	PHE	A	299	15.660	25.233	19.357	1.00
		2205 A	PHE	A	299	16.217	25.432	20.610	1.00
15		2206 A	PHE	A	299	15.436	25.929	21.642	1.00
		2207 A		A	299	12.200	28.872	23.504	1.00
20	ATOM 19.79		PHE	A	299	12.886	29.548	24.280	1.00
		2209 A	PRO	A	300	10.904	28.683	23.680	1.00
		2210 A	PRO	A	300	10.054	27.945	22.747	1.00
25		2211 A	PRO	Α	300	8.819	27.671	23.583	1.00
		2212 A	PRO	Α	300	8.712	28.898	24.513	1.00
30	ATOM 20.25		PRO	Α	300	10.120	29.311	24.758	1.00
		2214 A		<b>A</b>	300	9.672	28.834	21.581	1.00

	ATOM 21.44			PRO	A	300	9.921	30.043	21.655	1.00
		2216 A		ASN	A	301	9.076	28.282	20.524	1.00
5	ATOM 21.53			ASN	A	301	8.874	29.078	19.319	1.00
				ASN	A	301	10.198	29.173	18.567	1.00
10	ATOM 20.14			ASN	A	301	10.320	30.458	17.764	1.00
	ATOM 17.42			ASN	Α	301	9.875	30.553	16.607	1.00
		2221 A		ASN	A	301	10.920	31.454	18.371	1.00
15	ATOM 22.14			ASN	A	301	7.823	28.534	18.355	1.00
	ATOM 23.49			ASN	A	301	7.868	27.379	17.978	1.00
20	ATOM 22.24			GLY	A	302	6.970	29.416	17.854	1.00
		2225 A			A	302	5.912	29.031	16.932	1.00
	ATOM 20.83	2226 A	C C	GLY	A	302	6.292	29.165	15.475	1.00
25	ATOM 21.22	2227 A	0 0	GLY	A	302	5.574	28.669	14.603	1.00
			N N	ASN	Α	303	7.446	29.787	15.225	1.00
30		2229 A	CA C	ASN	A	303	7.981	30.005	13.886	1.00
	ATOM. 17.45	2230 A		ASN	A	303	8.705	31.349	13.816	1.00

		2231 A			A	303	7.872	32.473	14.381	1.00
	ATOM 21.34				Α	303	6.802	32.779	13.847	1.00
5	ATOM 22.58				A	303	8.305	33.033	15.530	1.00
		2234 A			A	303	8.926	28.922	13.414	1.00
10	ATOM 13.70				Α	303	8.831	28.481	12.239	1.00
		2236 A			Α	304	9.841	28.506	14.298	1.00
		2237 A			A	304	10.855	27.513	13.946	1.00
15		2238 A		GLN	A	304	12.235	28.005	14.316	1.00
		2239 A		GLN	A	304	12.556	27.976	15.811	1.00
20		2240 A		GLN	Α	304	14.020	28.087	16.123	1.00
		2241 A		GLN	A	304	14.842	27.582	15.386	1.00
	ATOM 9.76	2242 A	NE2 N	GLN	Α	304	14.352	28.794	17.223	1.00
25	ATOM 13.52		C C	GLN	A	304	10.601	26.128	14.582	1.00
	ATOM 13.66	2244 A		GLN	A	304	11.372	25.208	14.381	1.00
<b>30</b> ,	ATOM 12.81	2245 A	N N	GLY	<b>A</b>	305	9.537	25.972	15.343	1.00
	ATOM 12.54	2246 A	CA C	GLY	Α	305	9.351	24.745	16.101	1.00

	ATOM 12.99	2247 A		GLY	A	305	10.57	8 24.498	16.970	1.00
	ATOM 11.36	2248 A		GLY	A	305	11.06	2 25.409	17.633	1.00
5	ATOM 12.12	2249 A			A	306	11.10	7 23.272	16.926	1.00
	ATOM 12.07			TRP	A	306	12.28	6 22.898	17.701	1.00
10				TRP	A	306	12.13	0 21.473	18.254	1.00
	ATOM 11.34	2252 A	CG C	TRP	A	306	10.86	6 21.349	19.092	1.00
	ATOM 12.28	2253 A		TRP	A	306	9.75	5 20.611	18.805	1.00
15	ATOM 13.42			TRP	Α	306	8.81	2 20.766	19.794	1.00
	ATOM 12.23	2255 A		TRP	A	306	9.31	6 21.592	20.761	1.00
20	ATOM 13.78	2256 A	CD2 C	TRP	A	306	10.61	6 21.963	20.359	1.00
		2257 A		TRP	A	306	11.34	4 22.822	21.183	1.00
	ATOM 12.96	2258 A		TRP	A	306	10.78	0 23.247	22.365	1.00
25	ATOM 13.70	2259 A	CH2 C	TRP	A	306	9.48	8 22.854	22.735	1.00
	ATOM 14.65			TRP	A	306	8.74	4 22.035	21.945	1.00
30	ATOM 12.73	2261 A		TRP	A	306	13.56	2 23.046	16.890	1.00
	ATOM 14.46		0 0	TRP	A	306	14.63	2 22.620	17.318	1.00

		2263 A	GLY	A	307		13.479	23.716	15.741	1.00
		2264 A	GLY	A	307		14.679	24.111	15.015	1.00
5	ATOM 11.91	2265 A	GLY	A	307		14.871	23.392	13.685	1.00
		2266 A	GLY	A	307		14.008	22.628	13.238	1.00
10		2267 A	ARG	A	308		16.007	23.658	13.046	1.00
		2268 A	ARG	A	308		16.299	23.167	11.701	1.00
١		2269 A	ARG	A	308		17.153	24.223	10.961	1.00
15	ATOM 13.43	2270 A	ARG	A	308		17.388	23.970	9.462	1.00
	ATOM 13.61	2271 A	ARG	Α	308		18.284	25.025	8.807	1.00
20	ATOM 16.45	2272 A	ARG	А	308	-	19.563	25.031	9.510	1.00
		2273 A	ARG	A	308		20.127	26.086	10.086	1.00
		2274 A	ARG	A	308		21.257	25.902	10.762	1.00
25		2275 A	ARG	Α	308		19.660	27.319	9.902	1.00
		2276 A	ARG	A	308		17.055	21.837	11.770	1.00
30	ATOM 12.82	2277 A	ARG	Α	308		18.094	21.742	12.434	1.00
	ATOM 11.99		VAL	A	309		16.549	20.817		1.00

	ATOM 12.04	2279 A		VAL	A	309		17.170	19.498	11.096	1.00
	ATOM 11.35	2280 A		VAL	A	309		16.553	18.573	10.051	1.00
5		2281 A:		VAL	Α	309		17.354	17.272	9.961	1.00
		2282 A		VAL	Α	309		15.047	18.335	10.377	1.00
10	ATOM 12.28			VAL	Α	309		18.667	19.545	10.868	1.00
	ATOM 11.94			VAL	Α	309		19.148	20.157	9.930	1.00
		2285 A		THR	Α	310		19.393	18.904	11.760	1.00
15		2286 A		THR	Α	310		20.854	18.814	11.675	1.00
		2287 A		THR	Α	310		21.471	19.719	12.723	1.00
20			OG1		Α	310		21.044	21.090	12.516	1.00
	ATOM		CG2		Α			22.962	19.747	12.610	1.00
	MOTA		С	THR	Α	310		21.197	17.347	11.911	1.00
25	ATOM	2291 A	0	THR	Α	310		21.411	16.896	13.064	1.00
	ATOM	2292 A	N	LEU	Α	311		21.269	16.601	10.818	1.00
20	ATOM	2293	CA	LEU	Α	311		21.110	15.149	10.879	1.00
30	14.11 ATOM 13.67	2294 A		LEU	A	311	·	20.956	14.589	9.463	1.00

		2295 A		LEU	A	311		20.879	13.078	9.311	1.00
	ATOM 15.11			LEU .	A	311		19.749	12.522	10.109	1.00
5		2297 A			A	311		20.749	12.688	7.849	1.00
		2298 A		LEU	Α	·311		22.252	14.455	11.605	1.00
10				LEU	Α	311		22.012	13.521	12.345	1.00
•	ATOM 15.58	2300 A		ASP	Α	312		23.483	14.959	11.462	1.00
		2301 A		ASP .	A	312		24.624	14.307	12.111	1.00
15	ATOM 16.93			ASP .	A	312		25.984	14.797	11.582	1.00
	ATOM 19.05	2303 A		ASP .	A	312		26.222	16.245	11.822	1.00
20	ATOM 25.94	2304 A		ASP A	A	312	-	27.394	16.614	11.755	1.00
		2305 A		ASP A	A	312		25.348	17.090	12.090	1.00
	ATOM 16.48	2306 A	C C	ASP	A	312		24.560	14.330	13.615	1.00
25	ATOM 17.40	2307 A	0	ASP	Α	312		24.965	13.381	14.241	1.00
	ATOM 16.32	2308 A	N N	LYS	A	313		23.976	15.364	14.202	1.00
30	ATOM 16.35	2309 A		LYS A	A	313		23.755	15.366	15.641	1.00
	ATOM 17.66	2310 A	CB C	LYS A	Ą	313		23.363	16.773	16.130	1.00

	ATOM 20.65			LYS A	313	24.430	17.848	15.938	1.00
	ATOM 28.29	2312 A		LYS A	313	24.735	18.590	17.250	1.00
5	ATOM 31.10	2313 A		LYS A	313	25.619	17.746	18.162	1.00
	ATOM 32.31	2314 A		LYS A	313	26.458	18.529	19.131	1.00
10	ATOM 15.36			LYS A	313	22.666	14.379	16.100	1.00
	ATOM 15.49	2316 A		LYS A	313	22.662	13.968	17.258	1.00
			N N		314	21.755	14.007	15.212	1.00
15	ATOM 13.37			SER A	314	20.700	13.047	15.537	1.00
	ATOM 13.56	2319 A		SER A	314	19.497	13.217	14.590	1.00
20	ATOM 11.16	2320 A		SER A	314	18.889	14.489	14.723	1.00
		2321 A		SER A	314	21.148	11.581	15.505	1.00
	ATOM 14.30		0 0	SER A	314	20.507	10.717	16.112	1.00
25	ATOM 14.58	2323 A	N N	LEU A	315	22.209	11.285	14.771	1.00
	ATOM 15.64		CA C	LEU A	315	22.563	9.896	14.484	1.00
30	ATOM 15.15		CB C'	LEU A	315	23.750	9.824	13.505	1.00
``	ATOM 14.88		CG C	LEU A	315	23.506	10.436	12.143	1.00

	ATOM 16.67	2327 A		LEU	A	315		24.834	10.445	11.360	1.00
		2328 A		LEU	A	315		22.401	9.683	11.411	1.00
5	ATOM 16.16	2329 A			A	315		22.905	9.095	15.733	1.00
		2330 A		LEU	Α	315		22.442	7.956	15.894	1.00
10	ATOM 17.60			ASN	A	316		23.692	9.686	16.631	1.00
		2332 A		ASN	Α	316		24.235	8.915	17.749	1.00
		2333 A		ASN	A	316		25.757	8.837	17.694	1.00
15		2334 A		ASN	A	316		26.264	7.879	16.601	1.00
		2335 A		ASN	Α	316		25.736	6.732	16.397	1.00
20	ATOM 23.13	2336 A		ASN	Α	316		27.321	8.320	15.910	1.00
		2337 A		ASN	A	316		23.732	9.396	19.116	1.00
	ATOM 15.93	2338 A		ASN	Α	316		24.390	9.212	20.152	1.00
25			N N	VAL	Α	317		22.505	9.912	19.123	1.00
	ATOM 15.40	2340 A	CA C	VAL	A	317		21.820	10.220	20.389	1.00
30	ATOM		СВ	VAL	Α	317		20.360	10.675	20.150	1.00
			CG1	VAL	Α	317	·	20.335	11.940	19.350	1.00

		2343 A		VAL	Α	317	19.547	9.600	19.458	1.00
	ATOM 14.67	2344 A		VAL	A	317	21.803	8.995	21.323	1.00
5	ATOM 14.77			VAL	Α	317	21.675	7.864	20.868	1.00
	ATOM 13.95	2346 A		ALA	A	318	21.932	9.225	22.627	1.00
10	ATOM 13.64			ALA	A	318	21.623	8.186	23.603	1.00
	ATOM 13.50	2348 A		ALA	Α	318	22.196	8.523	24.940	1.00
	ATOM 13.19			ALA	A	318	20.087	8.130	23.652	1.00
15		2350 A	0 0	ALA	A	318	19.416	9.168	23.498	1.00
		2351 A		PHE	Α	319	19.512	6.952	23.853	1.00
20		2352 A		PHE	A	319	18.076	6.824	23.633	1.00
	ATOM 12.79	2353 A		PHE	Α	319	17.815	6.531	22.137	1.00
	ATOM 14.03	2354 A		PHE	A	319	18.267	5.158	21.700	1.00
25	ATOM 12.44	2355 A		PHE	Α	319	19.504	4.980	21.107	1.00
	ATOM 15.58			PHE	A	319	19,930	3.725	20.718	1.00
30	ATOM 15.26			PHE	Α	319	19.115	2.619	20.921	1.00
	ATOM 14.77		CE2 C	PHE	A	319	17.887	2.777	21.524	1.00

		2359 A	PHE	A	319	1	7.461	4.047	21.905	1.00
	ATOM 12.38	2360 A	PHE	A	319	1	7.349	5.799	24.461	1.00
5		2361 A		A	319	1	7.947	4.918	25.055	1.00
	ATOM 12.04			A	320	1	6.032	5.947	24.488	1.00
10	ATOM 12.42		VAL	A	320	1	5.125	4.909	24.949	1.00
		2364 A		Α	320	1	4.391	5.323	26.252	1.00
		2365 A	VAL	A	320	1	3.237	4.331	26.589	1.00
15	ATOM 13.91		VAL	A	320	1	5.401	5.395	27.416	1.00
	ATOM 11.88		VAL	A	320	1	4.137	4.758	23.802	1.00
20	ATOM 10.13		VAL	A	320	1	3.668	5.749	23.271	1.00
	ATOM 11.82		ASN	A	321	1	3.824	3.520	23.441	1.00
		2370 A	ASN	Α	321	1	3.018	3.205	22.261	1.00
25	ATOM 11.75		ASN	A	321	1	3.858	2.323	21.313	1.00
	ATOM 12.10		ASN	Α	321	1	3.214	2.117	19.944	1.00
30	ATOM 12.86		ASN	Α	321	1:	2.506	3.005	19.437	1.00
	ATOM 10.43		ASN	Α	321	1	3.451	0.919	19.328	1.00

	ATOM 12.63		C C	ASN	A	321	11.711	2.463	22.637	1.00
	ATOM 12.41	2376 A		ASN	A	321	11.509	1.311	22.260	1.00
5	ATOM 12.99		N N	GLU	A	322	10.835	3.130	23.380	1.00
	ATOM 13.23	2378 A		GLU	Α	322	9.542	2.552	23.760	1.00
10	ATOM 13.10	2379 A		GLU	Α	322	8.601	2.415	22.528	1.00
	ATOM 12.18	2380 A		GLU	Α	322	8.146	3.794	22.013	1.00
	ATOM 14.48	2381 A		GLU	Α	322	7.072	3.781	20.933	1.00
15	ATOM 15.20			GLU	A	322	6.747	4.884	20.429	1.00
	ATOM 14.00	2383 A		GLU	A	322	6.564	2.690	20.588	1.00
20	ATOM 14.04	2384 A		GLU	A	322	9.654	1.239	24.556	1.00
	ATOM 12.70	2385 A		GLU	A	322	8.778	0.385	24.468	1.00
	ATOM 13.33			THR	Α	323	10.688	1.122	25.387	1.00
25	ATOM 14.72	2387 A	CA C	THR	Α	323	10.907	-0.101	26.145	1.00
	ATOM 14.45	2388 A		THR	A	323	12.375	-0.466	26.173	1.00
30	ATOM 16.74	2389 A	OG1 O	THR	A	323	13.168	0.721	26.401	1.00
	ATOM 15.39	2390 A	CG2 C		A	323	12.813	-0.980	24.810	1.00

	ATOM 15.63	2391 A			2 A	323	10.397	-0.045	27.589	1.00
	ATOM 14.71	2392 A			2 A	323	10.572	-1.011	28.319	1.00
. 5	ATOM 15.41	2393 A			A	324	9.796	1.073	28.002	1.00
	ATOM 15.78	2394 A		SER	Α	324	9.176	1.159	29.341	1.00
10	ATOM 15.94	2395 A		SER	A	324	10.008	2.045	30.272	1.00
,		2396 A		SER	A	324	11.281	1.460	30.594	1.00
	ATOM 15.74	2397 A		SER	Α	324	7.739	1.723	29.257	1.00
15		2398 A		SER	A	324	7.558	2.937	29.315	1.00
	ATOM 16.08	2399 A		PRO	A	325	6.729	0.864	29.118	1.00
20		2400 A		PRO	A	325	5.326	1.306	29.170	1.00
	ATOM 17.76	2401 A		PRO	Α	325	4.525	0.035	28.823	1.00
		2402 A		PRO	Α	325	5.454	-1.106	29.084	1.00
25	ATOM 16.38	2403 A		PRO	A	325	6.845	-0.585	28.885	1.00
	ATOM 17.68	2404 A		PRO	A	325	4.926	1.815	30.548	1.00
30	ATOM 18.68	2405 A		PRO	A	325	5.277	1.211	31.553	1.00
•	ATOM 18.30	2406 A	N N	LEU	A	326	4.204	2.916	30.596	1.00

		2407 A		LEU	A	326	3.796	3.491	31.871	1.00
	ATOM 18.37	2408 A		LEU	A	326	4.410	4.890	32.059	1.00
5		2409 A		LEU	A	326	5.938	5.027	32.161	1.00
		2410 A		LEU	A	326	6.350	6.502	32.200	1.00
10	ATOM 17.55	2411 A		LEU	A	326	6.471	4.338	33.387	1.00
		2412 A			A	326	2.287	3.605	31.982	1.00
		2413 A		LEU	A	326	1.589	3.926	30.989	1.00
15		2414 A		SER	A	327	1.810	3.326	33.201	1.00
	ATOM 19.58	2415 A		SER	A	327	0.438	3.607	33.672	1.00
20		2416 A		SER	A	327	-0.123	2.391	34.397	1.00
		2417 A		SER	A	327	-0.176	1.357	33.434	1.00
	ATOM 19.58	2418 A	C C	SER	A	327	0.558	4.902	34.476	1.00
25	ATOM 18.88	2419 A	0 0	SER	A	327	1.609	5.154	35.075	1.00
,	ATOM 20.38	2420 A	N	THR	A	328	-0.505	5.696	34.595	1.00
30	ATOM 19.96	2421 A	CA C	THR	A	328	-0.861	6.454	35.789	1.00
	ATOM 20.43	2422 A	CB C	THR	A	328	-2.343	6.678	35.951	1.00

	ATOM 20.32	2423 A		328	-2.870	7.047	34.681	1.00
	ATOM 21.84			328	-2.602	7.922	36.842	1.00
5	ATOM 19.51	2425 A	C THR A	. 328	-0.102	6.262	37.084	1.00
		2426 A	O THR A	. 328	-0.223	5.222	37.739	1.00
10	ATOM 18.40			329	0.732	7.268	37.356	1.00
		2428 A		329	1.489	7.464	38.588	1.00
		2429 A	CB BSER A	329	0.679	7.017	39.818	0.50
		2430 A		329	0.629	7.141	39.833	0.50
		2431 A		329	0.653	5.599	39.887	0.50
	ATOM 20.52		OG ASER A	329	-0.672	7.722	39.718	0.50
		2433 A	C SER A	329	2.792	6.686	38.588	1.00
		2434 A	O SER A	329	3.533	6.753	39.550	1.00
25	ATOM 17.70		N GLN A	330	3.066	5.936	37.524	1.00
	ATOM 17.71	2436 A	CA GLN A	330	4.339	5.250	37.420	1.00
30	ATOM 17.37	2437 A	CB GLN A	330	4.193	4.001	36.566	1.00
	ATOM 17.60	2438 A	CG GLN A	330	3.233	2.970	37.168	1.00

	ATOM 18.11			GLN	A	330	3.116	1.700	36.319	1.00
	ATOM 16.08	2440 A		GLN	Α	330	3.305	1.763	35.119	1.00
5	ATOM 15.56			GLN	Α	330	2.762	0.550	36.952	1.00
	ATOM 18.14			GLN	Α	330	5.401	6.195	36.837	1.00
10	ATOM 18.07			GLN	A	330	5.103	7.308	36.423	1.00
-	ATOM 18.66			LYS	Α	331	6.643	5.750	36.842	1.00
	ATOM 19.23			LYS	A	331	7.710	6.524	36.276	1.00
15	ATOM 20.19			LYS	A	331	8.229	7.550	37.289	1.00
	ATOM 23.65			LYS	Α	331	8.972	6.934	38.450	1.00
20	ATOM 28.70			LYS	Α	331	9.071	7.912	39.625	1.00
	ATOM 31.64			LYS	Α	331	9.954	7.332	40.754	1.00
	ATOM 34.93	2450 A		LYS	Α	331	10.409	8.388	41.729	1.00
25	ATOM 18.87	2451 A		LYS	Α	331	8.804	5.589	35.820	1.00
	ATOM 18.18	2452 A		LYS	Α	331	8.887	4.410	36.261	1.00
30	ATOM 17.37	2453 A		ALA	A	332	9.587	6.091	34.873	1.00
	ATOM 17.82	2454 A	CA C	ALÀ	Α	332	10.797	5.406	34.412	1.00

		2455 A		ALA	A	332	10.689	5.068	32.941	1.00
	ATOM 17.33		C C	ALA	Α	332	11.991	6.324	34.650	1.00
5	ATOM 16.52				A	332	11.999	7.480	34.213	1.00
	ATOM 17.85				A	333	13.005	5.805	35.325	1.00
10	ATOM 17.61			THR	Α	333	14.108	6.643	35.784	1.00
	ATOM 18.03				Α	333	14.194	6.544	37.304	1.00
	ATOM 19.93			THR	Α	333	12.956	6.966	37.902	1.00
15	ATOM 18.18			THR	A	333	15.234	7.490	37.851	1.00
	ATOM 17.36				A	333	15.410	6.186	35.159	1.00
20	ATOM 17.40			THR	A	333	15.727	4.987	35.162	1.00
		2465 A		TYR	A	334	16.176	7.135	34.628	1.00
	ATOM 17.42	2466 A		TYR	A	334	17.437	6.840	33.986	1.00
25	ATOM 16.94	2467 A	CB C	TYR	Α	334	17.308	6.975	32.464	1.00
	ATOM 16.41	2468 A	CG C	TYR	Α	334	16.144	6.230	31.860	1.00
30	ATOM 14.43	2469 A		TYR	A	334	16.273	4.891	31.458	1.00
•				TYR	A	334	15.205	4.205	30.912	1.00

	ATOM 15.02		CZ TYR A	334	13.977	4.846	30.772	1.00
	ATOM 16.23		OH TYR A	334	12.929	4.188	30.216	1.00
5	ATOM 15.62		CE2 TYR A	334	13.819	6.147	31.153	1.00
	ATOM 16.76		CD2 TYR A	334	14.907	6.835	31.718	1.00
10	ATOM 17.66		C TYR A	334	18.542	7.767		1.00
	ATOM 16.79		O TYR A	334	18.279	8.840	34.991	1.00
	ATOM 17.44		N SER A	335	19.783	7.375	34.169	1.00
15	ATOM 18.62		CA SER A	335	20.939	8.218	34.442	1.00
	ATOM 18.54		CB BSER A	335	21.879	7.537	35.433	0.50
20	ATOM 18.59		CB ASER A	335	21.916	7.518	35.393	0.50
	ATOM 18.97		OG BSER A	335	22.697	6.585	34.783	0.50
	ATOM 19.43	2482 A	OG ASER A	335	21.316	7.174	36.629	0.50
25	ATOM 18.52	2483 A	C SER A	335	21.680	8.538	33.128	1.00
	ATOM 18.14		O SER A	335	21.698	7.720	32.221	1.00
30	ATOM 17.92		N PHE A	336	22.298	9.715	33.049	1.00
	ATOM 18.36		CA PHE A	336	23.115	10.092	31.911	1.00

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		2487 A	CB C	PHE	A	336	:	22.324	10.949	30.900	1.00
	ATOM 17.47			PHE	Α	336	:	23.150	11.401	29.753	1.00
5		2489 A		PHE	A	336	:	23.733	12.667	29.739	1.00
		2490 A		PHE	A	336	:	24.529	13.067	28.654	1.00
10	ATOM 18.35			PHE	A	336	:	24.749	12.198	27.591	1.00
	ATOM 18.49	2492 A		PHE	A	336	:	24.174	10.936	27.601	1.00
		2493 A		PHE	Α	336	2	23.386	10.543	28.681	1.00
15		2494 A		PHE	A	336	:	24.314	10.898	32.403	1.00
		2495 A		PHE	Α	336	:	24.159	11.810	33.195	1.00
20	ATOM 19.28	2496 A		THR	A	337	:	25.504	10.547	31.938	1.00
		2497 A		THR	A	337	2	26.733	11.219	32.364	1.00
	ATOM 20.11	2498 A		THR	Α	337	2	27.879	10.201	32.343	1.00
25	ATOM 19.75	2499 A		THR	Α	337	2	27.609	9.175	33.321	1.00
	ATOM 21.58	2500 A	CG2 C	THR	A	337	2	29.159	10.857	32.796	1.00
30	ATOM 20.14	2501 A	C C	THR	A	337	2	27.096	12.369	31.440	1.00
	ATOM 20.10	2502 A	0 0	THR	Α	337	2	27.266	12.163	30.253	1.00

	ATOM 19.74			ALA	A	338		27.181	13.571	32.000	1.00
	ATOM 20.23	2504 A		ALA	A	338		27.487	14.793	31.259	1.00
5	ATOM 19.43	2505 A		ALA	Α	338		26.468	15.858	31.588	1.00
	ATOM 20.94			ALA	A	338		28.881	15.292	31.633	1.00
10	ATOM 19.43			ALA	A	338		29.389	14.991	32.710	1.00
	ATOM 22.51	2508 A		GLN	A	339		29.503	16.042	30.741	1.00
		2509 A	CA Č	GLN	Α	339		30.750	16.711	31.070	1.00
15	ATOM 24.34			GLN	Α	339	·	31.893	16.162	30.230	1.00
	ATOM 29.11	2511 A		GLN	Α	339		32.591	14.904	30.726	1.00
20	ATOM 36.99	2512 A		GLN	Α	339		34.116	14.923	30.437	1.00
		2513 A		GLN	Α	339		34.841	13.991	30.825	1.00
	ATOM 36.90	2514 A		GLN	A	339		34.597	15.995	29.778	1.00
25	ATOM 23.27	2515 A	C C	GLN	A	339		30.543	18.167	30.722	1.00
	ATOM 23.02	2516 A		GLN	A	339		30.034	18.485	29.641	1.00
30	ATOM 22.60	2517 A	N N	ALA	A	340		30.922	19.061	31.619	1.00
	ATOM 22.71	2518 A	CA C	ALA	A	340		30.793	20.492	31.347	1.00

	ATOM 22.84	2519 A	CB C	АLА	A	340	31.311	21.296	32.535	1.00
	ATOM 22.30	2520 A	C C		A	340	31.524	20.916	30.076	1.00
5	ATOM 22.44	2521 A			A	340	32.474	20.270	29.650	1.00
	ATOM 23.38	2522 A		GLY	A	341	31.063	21.996	29.455	1.00
10			CA C	GLY	Α	341	31.738	22.554	28.283	1.00
	ATOM 24.15			GLY	A	341	30.989	22.425	26.956	1.00
	ATOM 24.10	2525 A		GLY	A	341	31.457	22.902	25.917	1.00
15	ATOM 24.05	2526 A		LYS	Α	342	29.829	21.774	26.970	1.00
		2527 A		LYS	A	342	29.038	21.637	25.743	1.00
20	ATOM 25.08	2528 A		LYS	A	342	29.643	20.545	24.861	1.00
	ATOM 27.13	2529 A		LYS	A	342	29.610	19.148	25.496	1.00
	ATOM 29.40	2530 A		LYS	Α	342	30.471	18.173	24.723	1.00
25	ATOM 29.96	2531 A		LYS	Α	342	30.254	16.725	25.182	1.00
	ATOM 32.09	2532 A		LYS	Α	342	30.738	16.515	26.576	1.00
30	ATOM 23.40	2533 A	C C	LYS	·A	342	27.552	21.373	26.058	1.00
	ATOM 23.54			LYS	Α	342	27.220	20.861	27.144	1.00

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	ATOM 22.09	2535 A		PRO	A	343		26.652	21.755	25.151	1.00
		2536 A		PRO	A	343		25.219	21.683	25.450	1.00
5	ATOM 21.58	2537 A		PRO	A	343		24.557	22.206	24.163	1.00
	ATOM 22.06			PRO	A	343		25.613	23.026	23.492	1.00
10	ATOM 22.30	2539 A		PRO	A	343		26.902	22.348	23.820	1.00
	ATOM 19.35			PRO	A	343		24.729	20.279	25.756	1.00
		2541 A		PRO	A	343		25.311	19.298	25.317	1.00
15	ATOM 18.12			LEU	A	344	f	23.645	20.223	26.521	1.00
	ATOM 17.07	2543 A		LEU	A	344		22.945	18.988	26.790	1.00
20		2544 A		LEU	A	344		23.019	18.680	28.278	1.00
	ATOM 16.96			LEU	A	344		22.250	17.476	28.788	1.00
	ATOM 16.29	2546 A	CD1 C	LEU	Α	344	,	22.743	16.188	28.128	1.00
25	ATOM 17.28	2547 A	CD2 C	LEU	Α	344	;	22.399	17.414	30.336	1.00
	ATOM 16.41	2548 A		LEU	Α	344		21.484	19.168	26.360	1,.00
30	ATOM 17.49	2549 A	0 0	LEU	Α	344		20.814	20.029	26.870	1.00
	ATOM 15.23	2550 A		LYS	A	345		21.013	18.336	25.440	1.00

		2551 A		LYS	A	345	19.638	18.405	24.943	1.00
		2552 A		LYS	A	345	19.644	18.807	23.474	1.00
<b>5</b>	ATOM 13.82	· 2553 A		LYS	A	345	20.104	20.235	23.248	1.00
		2554 A		LYS	A	345	19.987	20.664	21.795	1.00
10	ATOM 13.96			LYS	A	345	18.599	21.126	21.423	1.00
٠		2556 A		LYS	A	345	18.513	21.491	19.992	1.00
-	ATOM 14.25			LYS	A	345	18.929	17.066	25.135	1.00
15		2558 A		LYS	A	345	19.399	16.033	24.658	1.00
		2559 A		ILE	Α	346	17.821	17.084	25.870	1.00
20	ATOM 13.30			ILE	Α	346	17.031	15.888	26.116	1.00
		2561 A		ILE	Α	346	16.983	15.589	27.619	1.00
		2562 A		ILE	Α	346	18.376	15.444	28.197	1.00
25	ATOM 15.75	2563 A	CD1 C	ILE	Α	346	18.459	15.807	29.637	1.00
	ATOM 13.54	2564 A	CG2 C	ILE	A	346	16.180	14.329	27.874	1.00
30	ATOM 13.26	2565 A	C C	ILE	A	346	15.598	16.084	25.601	1.00
	ATOM 13.15	2566 A	0 0	ILE	Α	346	14.900	17.010	26.020	1.00

	ATOM 12.65			A	347	15.159	15.197	24.714	1.00
	ATOM 12.47			A	347	13.795	15.262	24.172	1.00
5	ATOM 12.36			A	347	13.838	15.473	22.654	0.35
		2570 A		A	347	13.813	15.524	22.662	0.65
10				A	347	12.569	15.297	22.042	0.35
	ATOM 13.18	2572 A		A	347	14.655	16.634	22.329	0.65
	ATOM 11.72	2573 A	C SER	A	347	13.032	13.983	24.491	1.00
15		2574 A		A	347	13.511	12.881	24.219	1.00
	ATOM 11.03			A	348	11.830	14.165	25.026	1.00
20	ATOM 10.93	2576 A	CA LEU C	A	348	10.864	13.121	25.289	1.00
		2577 A		A	348	10.302	13.274	26.706	1.00
	ATOM 10.80	2578 A		A	348	9.054	12.502	27.097	1.00
25		2579 A	CD1 LEU	Α	348	9.396	11.029	27.180	1.00
	ATOM 12.50	2580 A	CD2 LEU C	Α	348	8.542	12.969	28.443	1.00
30		2581 A	C LEU	Α	348	9.735	13.231	24.287	1.00
	ATOM 12.01	2582 A	O LEU	Α	348	9.152	14.302	24.140	1.00

	ATOM 10.58			A	349	9.389	12.127	23.631	1.00
	ATOM 11.32	2584 A	VAL	Α	349	8.327	12.142	22.638	1.00
5	ATOM 11.27			A	349	8.876	12.223	21.185	1.00
	ATOM 12.19		VAL	A	349	7.745	12.102	20.169	1.00
10	ATOM 11.93		VAL	A	349	9.653	13.511	20.961	1.00
	ATOM 11.68			A	349	7.522	10.873	22.768	1.00
	ATOM 12.43		VAL	A	349	8.099	9.802	22.870	1.00
15	ATOM 11.69		TRP	A	350	6.200	10.993	22.768	1.00
	ATOM 11.48		TRP	A	350	5.354	9.813	22.662	1.00
20	ATOM 11.79		TRP	A	350	4.719	9.442	24.002	1.00
	ATOM 11.11	2593 A	TRP	A	350	3.822	10.448	24.628	1.00
	ATOM 12.11	2594 A	TRP	Α	350	2.457	10.378	24.720	1.00
25	ATOM 12.24	2595 A	TRP	Α	350	1.961	11.469	25.386	1.00
	ATOM 13.16		TRP	A	350	3.015	12.262	25.774	1.00
30		2597 A	TRP	Α	350	4.208	11.640	25.311	1.00
	ATOM 12.51		TRP	Α	350	5.440	12.249	25.593	1.00

		2599 A		TRP	A	350	5.444	13.449	26.311	1.00
	ATOM 13.75	2600 A		TRP	A	350	4.248	14.022	26.767	1.00
5	ATOM 13.59	2601 A		TRP	A	350	3.022	13.427	26.507	1.00
		2602 A		TRP	A	350	4.314	9.883	21.536	1.00
10	ATOM 11.90			TRP	A	350	3.905	10.953	21.077	1.00
		2604 A		SER	A	351	3.921	8.707	21.071	1.00
		2605 A		SER	A	351	2.889	8.607	20.070	1.00
15		2606 A		SER	A	351	3.182	7.496	19.070	1.00
		2607 A		SER	A	351	4.356	7.772	18.310	1.00
20	ATOM 12.65			SER	A	351	1.636	8.378	20.884	1.00
		2609 A		SER	A	351	1.360	7.285	21.375	1.00
	ATOM 13.75	2610 A	N N	ASP	Α	352	0.947	9.477	21.115	1.00
25	ATOM 14.48	2611 A	CA C	ASP	Α	352	-0.205	9.532	21.982	1.00
	ATOM 14.84	2612 A	CB C	ASP	A	352	-0.508	11.003	22.225	1.00
30	ATOM 16.70	2613 A	CG C	ASP	A	352	-1.480	11.251	23.385	1.00
	ATOM 15.50	2614 A	OD1.	ASP	Α	352	-1.655	10.366	24.260	1.00

	ATOM 15.19	2615 A		ASP	Α	352		-2.115	12.329	23.458	1.00
	ATOM 15.19	2616 A		ASP	A	352		-1.427	8.842	21.389	1.00
5	ATOM 15.52	2617 A	0	ASP	<b>A</b>	352		-1.569	8.678	20.155	1.00
	ATOM 15.26	2618 A	N N	ALA	A	353		-2.331	8.434	22.273 -	1.00
10	ATOM 15.65	2619 A	CA C	ALA	A			-3.689	8.074	21.853	1.00
	ATOM 15.59	2620 A		ALA	A	353		-4.526	7.801	23.051	1.00
	ATOM 15.42	2621 A	C C	ALA	A	353		-4.325	9.197	21.018	1.00
15	ATOM 15.11	2622 A	0	ALA	A	353		-4.076	10.374	21.264	1.00
	ATOM 16.50		N N	PRO	A	354		-5.157	8.840	20.041	1.00
20	ATOM 16.92		CA C	PRO	A	354		-5.858	9.841	19.235	1.00
	ATOM 17.36	2625 A		PRO	A	354		-6.724	9.003	18.287	1.00
	ATOM 17.45		CG C	PRO	A	354		-6.790	7.646	18.897	1.00
25	ATOM 16.81	2627 A		PRO	À	354		-5.499	7.456	19.640	1.00
	ATOM 18.05	2628 A	C C	PRO	A	354		-6.723	10.771	20.073	1.00
30	ATOM 17.51	2629 A	0 0	PRO	A	354	·	-7.420	10.293	20.957	1.00
,	ATOM 18.60	2630 A	N N	GLY	A	355		-6.629	12.074	19.819	1.00

	ATOM 20.06			GLY	Α	355	-7	.392	13.071	20.527	1.00
	ATOM 21.21			GLY	A	355	-8	.773	13.285	19.936	1.00
5	ATOM 22.41			GLY	A	355	- 9	.095	12.758	18.880	1.00
	ATOM 22.87			SER	A	356	- 9	.598	14.050	20.628	1.00
10	ATOM 23.97			SER	A	356	-10	.939	14.377	20.145	1.00
	ATOM 24.97			SER	A	356	-11	.924	14.555	21.319	1.00
	ATOM 26.85	2637 A		SER	A	356	-12	.771	15.696	21.117	1.00
15	ATOM 24.04			SER	A	356	-10	.901	15.654	19.320	1.00
	ATOM 23.54			SER	A	356	-10	.151	16.583	19.635	1.00
20	ATOM 24.61			THR	A	357	-11	.714	15.684	18.261	1.00
		2641 A		THR	Α	357	-11	.826	16.846	17.396	1.00
				THR	A	357	-12	.423	16.436	16.032	1.00
25	ATOM 25.91	2643 A	OG1 O	THR	Α	357	-13	.673	15.748	16.218	1.00
	ATOM 25.30	2644 A	CG2 C	THR	Α	357	-11	.534	15.392	15.334	1.00
30	ATOM 26.58	2645 A		THR	A	357	-12	.687	17.982	18.000	1.00
	ATOM 26.22	2646 A	0	THR	A	357	-12	.812	19.035	17.398	1.00

	ATOM 27.59	2647 A		THR	A	358	-13.276	17.771	19.175	1.00
	ATOM 28.37			THR	A	358	-14.113	18.816	19.779	1.00
5	ATOM 28.27	2649 A		THR	Α	358	-15.575	18.335	19.938	1.00
	ATOM 28.60	2650 A		THR	Α	358	-15.606	17.065	20.606	1.00
10	ATOM 27.97			THR	Α	358	-16.192	18.066	18.587	1.00
	ATOM 28.71	2652 A		THR	A	358	-13.605	19.321	21.118	1.00
		2653 A		THR	À	358	-13.954	20.424	21.524	1.00
15	ATOM 28.63	2654 A		ALA	A	359	-12.758	18.548	21.795	1.00
		2655 A		ALA	A	359	-12.311	18.925	23.133	1.00
20	ATOM 28.64	2656 A		ALA	A	359	-11.668	17.739	23.814	1.00
		2657 A		ALA	A	359	-11.349	20.100	23.099	1.00
	ATOM 27.61	2658 A	0 0	ALA	A	359	-10.738	20.393	22.060	1.00
25	ATOM 27.18	2659 A	N N	SER	A	360	-11.213	20.785	24.241	1.00
	ATOM 27.00	2660 A	CA C	SER	A	360	-10.301	21.916	24.344	1.00
30		2661		SER	Α	360	-10.351	22.564	25.737	1.00
	ATOM 31.54	,		SER	A	360	-11.688	22.840	26.125	1.00

	ATOM 25.14			SER	A	360	-8.858	21.485	24.060	1.00
	ATOM 24.27			SER	A	360	-8.115	22.230	23.446	1.00
5	ATOM 23.74			LEU	A	361	-8.478	20.307	24.553	1.00
	ATOM 23.54			LEU	Α	361	-7.100	19.812	24.453	1.00
10	ATOM 23.87			LEU	A	361	-6.480	19.583	25.840	1.00
		2668	CG	LEU	A	361	-6.119	20.802	26.702	1.00
		2669	CD1	LEU	A	361	-5.434	20.335	27.980	1.00
15		2670	CD2	LEU	A	361	-5.217	21.827	25.975	1.00
	MOTA		С	LEU	Α	361	-7.097	18.493	23.701	1.00
22		2672	0	LEU	Α	361	-7.942	17.611	23.961	1.00
20	21.73 ATOM	2673	N	THR	A	362	-6.141	18.325	22.790	1.00
	19.81 ATOM		CA	THR	A	362	-6.053	17.058	22.066	1.00
25	18.76 ATOM	A 2675	C CB	THR	A	362	-5.433	17.230	20.657	1.00
	19.42 ATOM	A 2676	C OG1	THR	A	362	-4.100	17.707	20.786	1.00
	17.51	A	0				-6.174 .	18.305	19.862	1.00
30	20.58	A	С					16.023		1.00
	ATOM 17.21	2678 A		THK	А	302	- 201	10.025		

	ATOM 13.79			THR	A	362	-5.411	14.858	22.530	1.00
	ATOM 16.68	2680 A		LEU	A	363	-4.398	16.448	23.761	1.00
5	ATOM 16.39	2681 A		LEU	A	363	-3.560	15.505	24.484	1.00
	ATOM 16.30			LEU	A	363	-2.547	16.213	25.411	1.00
10	ATOM 16.62			LEU	A	363	-1.460	15.318	25.990	1.00
	ATOM 16.31			LEU	A	363	-0.380	14.960	24.939	1.00
	ATOM 15.84	2685 A		LEU	A	363	-0.838	15.936	27.236	1.00
15	ATOM 17.11			LEU	A	363	-4.424	14.536	25.280	1.00
	ATOM 17.15			LEU	A	363	-5.404	14.936	25.911	1.00
20	ATOM 16.50			VAL	A	364	-4.068	13.253	25.249	1.00
	ATOM 16.09	2689 A		VAL	A	364	-4.829	12.263	25.975	1.00
	ATOM 15.79	2690 A		VAL	A	364	-5.285	11.121	25.030	1.00
25	ATOM 17.24	2691 A		VAL	Α	364	-5.871	9.933	25.826	1.00
		2692 A	CG2 C	VAL	Α	364	-6.288	11.651	24.020	1.00
30	ATOM 15.68		C C	VAL	A	364	-3.983	11.744	27.139	1.00
		2694 A		VAL	Α	364	-4.329	11.942	28.309	1.00

		2695 A		ASN	A	365	-2.875	11.085	26.809	1.00
		2696 A		ASN	A	365	-1.931	10.614	27.804	1.00
5		2697 A			A	365	-1.302	9.286	27.354	1.00
		2698 A		ASN	Α	365	-2.342	8.161	27.214	1.00
10		2699 A		ASN	A	365	-3.298	8.081	28.004	1.00
		2700 A		ASN	A	365	-2.158	7.283	26.206	1.00
		2701 A		ASN	Α	365	-0.858	11.690	28.088	1.00
15		2702 A		ASN	Α	365	-0.174	12.190	27.172	1.00
	ATOM 14.06	2703 A		ASP	Α	366	-0.696	12.015	29.360	1.00
20		2704 A		ASP '	A	366	0.158	13.115	29.783	1.00
		2705 A		ASP	Α	366	-0.632	14.068	30.672	1.00
	ATOM 15.13	2706 A	CG C	ASP	Α	366	0.105	15.346	30.990	1.00
25	ATOM 13.15	2707 A	OD1 O	ASP	A	366	1.344	15.467	30.710	1.00
	ATOM 17.79	2708 A	OD2 O	ASP	A	366	-0.491	16.284	31.609	1.00
30	ATOM 14.89	2709 A	C C	ASP	Α	366	1.367	12.568	30.548	1.00
-	ATOM 15.57	2710 A	0 0	ASP	Α	366	1.257	12.132	31.708	1.00

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		2727 A		LEU A	369	8.603	15.108	31.520	1.00
	ATOM 14.31			LEU A	369	10.044	14.937	31.645	1.00
5	ATOM 13.72	2729 A		LEU A	369	10.735	15.448	30.380	1.00
	ATOM 12.96	2730 A		LEU A	369	12.238	15.284	30.298	1.00
10	ATOM 12.52			LEU A	. 369	12.572	13.850	30.345	1.00
	ATOM 14.11	2732 A		LEU A	. 369	12.749	15.953	28.980	1.00
		2733 A		LEU A	369	10.539	15.733	32.854	1.00
15		2734 A		LEU A	A 369	10.218	16.922	33.012	1.00
		2735 A		VAL A	A 370	11.315	15.085	33.698	1.00
20		2736 A		VAL A	370	11.875	15.729	34.905	1.00
٠		2737 A		VAL A	370	11.144	15.278	36.180	1.00
	ATOM 17.73	2738 A	CG1 C	VAL A	370	11.679	16.020	37.425	1.00
25	ATOM 15.57	2739 A	CG2 C	VAL A	370	9.687	15.487	36.024	1.00
	ATOM 15.46	2740 A	C C	VAL A	370	13.359	15.388	34.975	1.00
30	ATOM 15.96	2741 A	0 0	VAL A	370	13.767	14.219	35.042	1.00
	ATOM 15.15	2742 A	N N	ILE A	371	14.174	16.422	34.908	1.00

	ATOM 14.98			A	371		15.608	16.261	34.858	1.00
		2744 A	ILE A	A	371		16.171	17.036	33.669	1.00
5	ATOM 14.63		ILE A	A	371		15.509	16.589	32.336	1.00
		2746 A	ILE A	A	371		15.600	15.075	32.072	1.00
10			ILE A	Ą	371		17.674	16.922	33.614	1.00
		2748 A	ILE .	A	371		16.145	16.835	36.155	1.00
		2749 A	ILE .	A	371		15.648	17.853	36.618	1.00
15	ATOM 16.86	2750 A	THR .	A	372		17.150	16.174	36.727	1.00
	ATOM 17.19		THR 2	A	372	•	17.858	16.671	37.897	1.00
20	ATOM 17.36	2752 A	THR Z	A	372		17.618	15.748	39.089	1.00
	ATOM 18.17		THR A	A	372		16.212	15.514	39.265	1.00
	ATOM 17.84	2754 A	THR A	A	372		18.044	16.409	40.372	1.00
25	ATOM 17.65		THR .	A	372		19.364	16.729	37.634	1.00
	ATOM 18.44	2756 A	THR .				19.962	15.725	37.262	1.00
30	ATOM 17.80	2757 A	ALA .		373		19.971	17.891	37.870	1.00
	ATOM 18.13	2758 A	ALA i	Ą	373		21.376	18.118	37.606	1.00

		2759 A	CB C	ALA	A	373	21.643	19.607	37.475	1.00
	ATOM 19.16	2760 A		ALA	A	373	22.175	17.545	38.767	1.00
5	ATOM 18.57			ALA	A	373	21.601	17.188	39.780	1.00
		2762 A		PRO	Α	374	23.479	17.368	38.581	1.00
10		2763 A		PRO	Α	374	24.348	16.857	39.642	1.00
	ATOM 20.60	2764 A		PRO	A	374	25.727	16.884	39.001	1.00
	ATOM 20.96	2765 A		PRO	A	374	25.434	16.700	37.530	1.00
15		2766 A		PRO	À	374	24.174	17.460	37.286	1.00
	ATOM 22.06	2767 A	C C	PRO	Α	374	24.266	17.647	40.948	1.00
20	ATOM 23.95	2768 A		PRO	A	374	24.303	17.039	42.011	1.00
		2769 A		ASN	Α	375	24.024	18.954	40.873	1.00
	ATOM 23.32	2770 A	CA C	ASN	A	375	23.910	19.770	42.058	1.00
25	ATOM 24.03	2771 A	CB C	ASN	Α	375	24.515	21.165	41.790	1.00
	ATOM 26.93	2772 A	CG C	ASN	A	375	23.581	22.096	40.993	1.00
30	ATOM 28.51	2773 A	OD1 O	ASN	Α	375	22.515	21.689	40.492	1.00
	ATOM			ASN	Α	375	23.987	23.362		1.00

	ATOM 23.07	2775 A	C C	ASN A	375	22	.471	19.898	42.563	1.00
	ATOM 22.92			ASN A	375	22	.208	20.711	43.430	1.00
5	ATOM		_	GLY A	376	21	.541	19.120	42.010	1.00
	ATOM 21.43	2778 A	CA C	GLY A	376	20	.166	19.165	42.469	1.00
10		2779 A	C C	GLY A	376	19	.197	20.077	41.724	1.00
	ATOM 19.94		0 0	GLY A	376	17	.990	20.006	41.937	1.00
		2781 A	N N	THR A	377	. 19	.696	20.909	40.828	1.00
15	ATOM 21.36	2782 A	CA C	THR A	377	18	.793	21.785	40.090	1.00
	ATOM 21.19	2783 A		THR A	377	19	.571	22.738	39.220	1.00
20	ATOM 22.26	2784 A		THR A	377	20	.423	23.532	40.054	1.00
		2785 A		THR A	377	18	.635	23.724	38.538	1.00
	ATOM 20.56	2786 A	C C	THR A	377	17	.818	20.971	39.239	1.00
25	ATOM 19.93	2787 A	0	THR A	377	18	.206	20.058	38.541	1.00
	ATOM 20.68	2788 A	N N	LYS A	378	16	.558	21.345	39.315	1.00
30	ATOM 21.64	2789 A	CA C	LYS A	378	15	.488	20.630	38.644	1.00
	ATOM 22.42	2790 A	CB C	LYS A	378	14	.321	20.503	39.594	1.00

	ATOM 28.13	2791 A		LYS	A	378	13.709	19.168	39.611	1.00
	ATOM 33.32	2792 A		LYS	A	378	14.144	18.449	40.913	1.00
5	ATOM 34.92	2793 A		LYS	Α	378	13.743	17.001	40.854	1.00
	ATOM 38.61		NZ N	LYS	A	378	14.605	16.111	41.699	1.00
10		2795 A		LYS	A	378	14.990	21.344	37.397	1.00
	ATOM 19.59	2796 A		LYS	A	378	14.902	22.553	37.388	1.00
		2797 A	N N	TYR	A	379	14.623	20.568	36.378	1.00
15	ATOM 17.87	2798 A		TYR	Α	379	14.009	21.088	35.155	1.00
		2799 A		TYR	A	379	15.030	21.111	34.011	1.00
20	ATOM 17.53	2800 A		TYR	A	379	16.382	21.654	34.386	1.00
		2801 A		TYR	A	379	17.297	20.864	35.052	1.00
	ATOM 19.05	2802 A	CE1 C	TYR	Α	379	18.537	21.352	35.417	1.00
25	ATOM 21.25	2803 A	CZ C	TYR	A	379	18.895	22.655	35.097	1.00
	ATOM 20.46	2804 A	ОН	TYR	Α	379	20.160	23.104	35.465	1.00
30	ATOM 19.58			TYR	Α	379	18.004	23.459	34.399	1.00
	ATOM 18.07	2806 A	CD2 C	TYR	Α	379	16.751	22.953	34.060	1.00

	ATOM 17.42		TYR	A	379	12.852	20.198	34.732	1.00
	ATOM 18.13		TYR	A	379	12.967	18.973	34.766	1.00
5	ATOM 16.44		VAL	A	380	11.732	20.787	34.340	1.00
	ATOM 16.11		VAL	A	380	10.653	19.989	33.750	1.00
10			VAL	A	330	9.320	20.114	34.514	1.00
	ATOM 17.64		VAL	Α	380	9.521	19.742	36.000	1.00
	ATOM 16.52	2813 A	VAL	Α	380	8.716	21.505	34.369	1,00
15		2814 A	VAL	A	380	10.466	20.353	32.283	1.00
	ATOM 15.17		VAL	A	380	10.876	21.425	31.826	1.00
20	ATOM 14.19	2816 A	GLY	Α	381	9.868	19.436	31.547	1.00
	ATOM 13.85	2817 A	GLY	A	381	9.761	19.541	30.101	1.00
	ATOM 13.74	2818 A	GLY	A	381	9.132	20.847	29.647	1.00
25	ATOM 13.57		GLY	Α	381	8.096	21.259	30.153	1.00
	ATOM 13.87	2820 A	ASN	Α	382	9.813	21.509	28.729	1.00
30	ATOM 14.08		ASN	A	382	9.332	22.719	28.064	1.00
	ATOM 13.91	2822 A	ASN	Α	382	8.002	22.451	27.344	1.00

		2823 A		ASN	A	382	8.148	21.436	26.209	1.00
	ATOM 13.23	2824 A		ASN	Α	382	9.250	21.181	25.757	1.00
5	ATOM 10.67	2825 A		ASN	Α	382	7.041	20.850	25.770	1.00
		2826 A		ASN	A	382	9.232	23.942	28.966	1.00
10	ATOM 14.15			ASN	A	382	8.682	24.981	28.556	1.00
		2828 A -		ASP	A	383	9.796	23.869	30.178	1.00
		2829 A		ASP	A	383	9.813	25.057	31.017	1.00
15	ATOM 15.34			ASP	A	383	9.593	24.709	32.499	1.00
	ATOM 15.81	2831 A		ASP	Α	383	9.580	25.952	33.388	1.00
20	ATOM 16.83			ASP	Α	383	9.786	27.082	32.845	1.00
	ATOM 15.84	2833 A		ASP	Α	383	9.394	25.897	34.636	1.00
	ATOM 15.13	2834 A		ASP	A	383	11.127	25.813	30.810	1.00
25	ATOM 15.46			ASP	Α	383	12.160	25.490	31.398	1.00
	ATOM 15.11	2836 A		PHE	Α	384	11.074	26.859	30.000	1.00
30	•	2837	CA	PHE	Α	384	12.284	27.559	29.589	1.00
		2838	СВ	PHE	Α	384	12.178	27.818	28.086	1.00

				PHE	Α	384	12.247	26.560	27.240	1.00
	14.23	A								
	ATOM 19.41	2840 A		PHE	A	384	13.440	25.910	27.059	1.00
5	ATOM 19.08	2841 A		PHE	A	384	13.516	24.782	26.273	1.00
		2842 A		PHE	Α	384	12.395	24.303	25.685	1.00
10	ATOM 14.73			PHE	A	384	11.208	24.943	25.845	1.00
		2844 A		PHE	A	384	11.140	26.070	26.602	1.00
		2845 A		PHE	Α	384	12.546	28.857	30.389	1.00
15	ATOM 15.13	_		PHE	Α	384	13.547	29.558	30.152	1.00
		2847 A		THR	Α	385	11.666	29.151	31.350	1.00
20		2848 A		THR	A	385	11.820	30.294	32.264	1.00
		2849 A		THR	A	385	10.519	31.097	32.400	1.00
	ATOM 17.98		OG1 O	THR :	A	385	9.520	30.295	33.030	1.00
25	ATOM 18.21	2851 A		THR 2	A	385	9.922	31.491	31.028	1.00
	ATOM 17.95	2852 A	C C	THR	A	385	12.238	29.868	33.689	1.00
30	ATOM 17.41	2853 A	0 0	THR	Α	385	11.703	28.890	34.252	1.00
	ATOM 18.54	2854 A	N N	ALA	Α	386	13.197	30.599	34.250	1.00

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	ATOM 19.43	2855 A		ALA	Α	386		13.743	30.266	35.565	1.00
	ATOM 19.87			ALA	A	386		15.056	30.971	35.792	1.00
5	ATOM 20.06	2857 A			A	386		12.728	30.697	36.594	1.00
		2858 A		ALA	A	386		12.078	31.735	36.409	1.00
10	ATOM 19.71			PRO	A	387		12.525	29.897	37.635	1.00
		2860 A		PRO	Α	387		13.134	28.582	37.766	1.00
	ATOM 20.90	2861 A		PRO	A	387		12.951	28.269	39.250	1.00
15	ATOM 20.16	2862 A		PRO	Α	387		11.609	28.910	39.587	1.00
		2863 A		PRO	Α	387		11.670	30.223	38.796	1.00
20	ATOM 19.33			PRO	Α	387		12.413	27.549	36.890	1.00
	ATOM 18.07	2865 A	0 ,	PRO	Α	387		11.237	27.688	36.612	1.00
	ATOM 19.24	2866 A		TYR	A	388		13.144	26.521	36.491	1.00
25	ATOM 19.24	2867 A		TYR	A	388	£	12.781	25.672	35.365	1.00
	ATOM 18.91			TYR	A	388		14.059	25.211	34.661	1.00
30	ATOM 18.51	2869 A		TYR	A	388		14.912	26.363	34.177	1.00
	ATOM			TYR	A	388		16.128	26.625	34.761	1.00

		2871 A		TYR	A	388	16.912	27.701	34.350	1.00
	ATOM 15.12	2872 A		TYR	A	388	16.462	28.511	33.312	1.00
5		2873 A		TYR	A	388	17.242	29.565	32.918	1.00
		2874 A		TYR	A	388	15.241	28.276	32.723	1.00
10	ATOM 14.33			TYR	A	388	14.462	27.229	33.154	1.00
	ATOM 19.73	2876 A		TYR	A	388	11.934	24.467	35.745	1.00
		2877 A		TYR	A	388	11.688	23.598	34.913	1.00
15		2878 A		ASP	Α	389	11.422	24.442	36.972	1.00
	ATOM 21.41	2879 A		ASP	A	389	10.605	23.327	37.430	1.00
20		2880 A		ASP	Α	389	11.346	22.547	38.507	1.00
		2881 A		ASP	Α	389	11.504	23.343	39.796	1.00
	ATOM 27.95	2882 A		ASP	A	389	11.618	22.706	40.869	1.00
25	ATOM 24.63	2883 A	OD2 O	ASP	A	389	11.523	24.595	39.822	1.00
	ATOM 21.64	2884 A		ASP	A	389	9.246	23.724	37.968	1.00
30	ATOM 22.12		0	ASP	Α	389	8.629	22.947	38.709	1.00
	ATOM				Α	390	8.759	24.908	37.618	1.00

		2887 A		ASN	Α	390	7.455	25.326	38.130	1.00
		2888 A		ASN	A	390	7.555	26.664	38.892	1.00
5	ATOM 23.08	2889 A		ASN	A	390	7.965	27.825	37.989	1.00
		2890 A		ASN	A	390	8.404	27.620	36.847	1.00
10	ATOM 23.21	2891 A		ASN	Α	390	7.816	29.050	38.491	1.00
		2892 A			Α	390	6.356	25.402	37.060	1.00
		2893 A		ASN	A	390	5.181	25.500	37.405	1.00
15		2894 A		ASN	A	391	6.717	25.340	35.772	1.00
		2895 A		ASN	A	391	5.705	25.411	34.713	1.00
20	ATOM 21.22	2896 A		ASN	Α	391	5.986	26.567	33.728	1.00
		2897 A			A	391	6.221	27.924	34.426	1.00
	ATOM 22.21		OD1 O	ASN	A	391	7.345	28.481	34.388	1.00
25	ATOM 23.08	2899 A	ND2 N	ASN	Α	391	5.151	28.490	35.029	1.00
	ATOM 20.79	2900 A	C C	ASN	A	391	5.611	24.072	33.978	1.00
30	ATOM 21.08	2901 A	0 0	ASN	A	391	6.295	23.818	32.978	1.00
	ATOM 20.10	2902 A	N N	TRP	Α	392	4.741	23.211	34.467	1.00

	ATOM 20.04	2903 A		TRP	Α	392	4.601	21.862	33.928	1.00
	ATOM 20.74	2904 A		TRP	Α	392	3.893	20.979	34.926	1.00
5	ATOM 24.30	2905 A		TRP	A	392	4.629	20.757	36.231	1.00
	ATOM 28.54			TRP	A	392	4.687	21.605	37.309	1.00
10	ATOM 30.71	2907 A		TRP	Α	392	5.435	21.038	38.317	1.00
	ATOM 28.29	2908 A		TRP	Α	392	5.870	19.804	37.902	1.00
	ATOM 27.17			TRP	Α	392	5.367	19.594	36.598	1.00
15	ATOM 29.38			TRP	A	392	5.695	18.400	35.937	1.00
	ATOM 28.54			TRP	A	392	6.456	17.447	36.608	1.00
20	ATOM 30.49			TRP	A	392	6.922	17.683	37.904	1.00
	ATOM 30.31	2913 A		TRP	<b>A</b>	392	6.643	18.857	38.566	1.00
	ATOM 19.03	2914 A	C C	TRP	A	392	3.767	21.890	32.661	1.00
25	ATOM 19.40	2915 A	0 0	TRP	A	392	2.828	22.678	32.552	1.00
	ATOM 17.66	2916 A	N N	ASP	A	393	4.107	21.020	31.709	1.00
30	ATOM 16.59	2917 A	CA C	ASP	A	393	3.416	20.958	30.424	1.00
	ATOM 16.47	2918 A	CB C	ASP	A	393	4.431	20.669	29.332	1.00

	ATOM 15.80	2919 A		ASP	Α	393	3.813	20.660	27.930	1.00
	ATOM 14.98	2920 A		ASP	Α	393	4.350	21.364	27.045	1.00
5	ATOM 15.12	2921 A		ASP	A	393	2.817	19.975	27.629	1.00
	ATOM 16.46	2922 A		ASP	Α	393	2.324	19.888	30.425	1.00
10	ATOM 15.65			ASP	A	393	2.606	18.716	30.648	1.00
	ATOM 15.96	2924 A		GLY	A	394	1.080	20.302	30.178	1.00
		2925 A		GLY	A	394	-0.029	19.384	30.014	1.00
15		2926 A		GLY	A	394	-0.747	19.498	28.675	1.00
		2927 A		GLY	A	394	-1.936	19.255	28.601	1.00
20	ATOM 17.31	2928 A		ARG	A	395	-0.030	19.864	27.617	1.00
	ATOM 17.68	2929 A		ARG	Α	395	-0.607	19.978	26.264	1.00
	ATOM 19.08	2930 A	CB C	ARG	A	395	-0.588	21.437	25.783	1.00
25	ATOM 26.02	2931 A	CG C	ARG	A	395	-1.434	22.408	26.518	1.00
	ATOM 31.34	2932 A	CD C	ARG	A	395	-1.172	23.839	26.066	1.00
30	ATOM 37.30	2933 A	NE N	ARG	Α	395	-1.802	24.813	26.969	1.00
	ATOM 40.58	2934 A		ARG	Α	395	-3.026	25.331	26.821	1.00

	ATOM 44.12		ARG	Α	395	-3.478	26.216	27.717	1.00
	ATOM 40.20		ARG	A	395	-3.805	24.983	25.805	1.00
5	ATOM 15.80		ARG	Α	395	0.176	19.240	25.165	1.00
	ATOM 16.01		ARG	A	395	-0.418	18.827	24.176	1.00
10	ATOM 14.41		ASN	A	396	1.502	19.212	25.282	1.00
	ATOM 13.89		ASN	A	396	2.389	18.645	24.251	1.00
	ATOM 13.10	2941 A	ASN	A	396	3.662	19.483	24.133	1.00
15	ATOM 14.63		ASN	A	396	3.408	20.889	23.585	1.00
	ATOM 11.53		ASN	A	396	3.129	21.075	22.374	1.00
20	ATOM 11.89		ASN	A	396	3.550	21.897	24.463	1.00
	ATOM 13.64		ASN	A	396	2.806	17.197	24.475	1.00
	ATOM 14.92	2946 A	ASN	A	3.96	2.995	16.743	25.634	1.00
25	ATOM 13.56		ASN	A	397	2.973	16.452	23.376	1.00
		2948 A	ASN	A	397	3.539	15.085	23.451	1.00
30	ATOM 12.41		ASN	A	397	2.705	14.080	22.672	1.00
	ATOM 13.07				397	2.539	14.450	21.192	1.00

		2951 A		ASN	A	397		2.243	15.594	20.849	1.00
	ATOM 13.08			ASN	A	397		2.683	13.466	20.324	1.00
5	ATOM 13.13	2953 A		ASN	A	397		5.011	15.077	23.010	1.00
		2954 A		ASN	A	397		5.607	14.010	22.663	1.00
10	ATOM 12.66				Α	398		5.577	16.291	23.028	1.00
	ATOM 12.58			VAL	A	398	·	6.992	16.524	22.914	1.00
	ATOM 13.06	2957 A		VAL	A	398		7.329	17.261	21.626	1.00
15	ATOM 11.41	2958 A		VAL	Α	398		8.835	17.523	21.533	1.00
	ATOM 12.98	2959 A		VAL	A	398		6.846	16.476	20.408	1.00
20	ATOM 12.92				A	398		7.381	17.412	24.105	1.00
		2961 A		VAL	A	398		6.819	18.501	24.272	1.00
	ATOM 12.47	2962 A	N N	GLU	A	399		8.288	16.913	24.945	1.00
25	ATOM 12.81	2963 A	CÀ C		A			8.797	17.666	26.107	1.00
	ATOM 12.40	2964 A	CB C	GLU	Α	399		8.339	17.054	27.452	1.00
30	ATOM 11.56	2965 A	CG C	GLU	Α	399		6.870	17.340	27.793	1.00
	ATOM 13.58	2966 A	CD C	GLU	A	399	,	6.538	17.357	29.284	1.00

	ATOM 14.48	2967 A		GLU	A	399	5.312	17.324	29.635	1.00
	ATOM 14.20	2968 A		GLU	A	399	7.471	17.421	30.112	1.00
5	ATOM 12.44	2969 A			A	399	10.307	17.680	26.052	1.00
		2970 A		GLU	A	399	10.920	16.624	25.929	1.00
10	ATOM 12.69			ASN	Α	400	10.890	18.883	26.174	1.00
	ATOM 12.36			ASN	Α	400	12.326	19.098	26.073	1.00
	ATOM 12.37			ASN	A	400	12.636	19.953	24.822	1.00
15	ATOM 14.26			ASN	Α	400	12.185	19.302	23.559	1.00
	ATOM 16.94			ASN	A	400	12.621	18.213	23.247	1.00
20	ATOM 14.56	2976 A		ASN	A	400	11.302	19.964	22.817	1,00
		2977 A		ASN	A	400	12.959	19.820	27.254	1.00
	ATOM 11.03	2978 A		ASN	A	400	12.363	20.716	27.867	1.00
25			N N	VAL	Α	401	14.200	19.448	27.543	1.00
	ATOM 11.67	2980 A	CA C	VAL	Α	401	15.042	20.183	28.494	1.00
30		2981 A	CB C	VAL	A	401	15.230	19.394	29.804	1.00
	ATOM 13.18	2982 A	CG1 C	VAL	Α	401	16.317	20.017	30.668	1.00

		2983 A		VAL 2	A	401	13.962	19.359	30.558	1.00
	ATOM 12.10			VAL	A	401	16.351	20.372	27.792	1.00
5		2985 A		VAL	A	401	17.022	19.394	27.471	1.00
		2986 A		PHE	A	402	16.693	21.634	27.528	1.00
10				PHE .	A	402	17.841	22.019	26.744	1.00
	ATOM 14.70			PHE .	A	402	17.401	22.853	25.517	1.00
		2989 A		PHE .	A	402	16.602	22.079	24.464	1.00
15	ATOM 15.18			PHE Z	A	402	15.936	22.764	23.455	1.00
	ATOM 12.37			PHE 2	A	402	15.222	22.069	22.468	1.00
20	ATOM 11.68	2992 A		PHE 2	A	402	15.195	20.700	22.489	1.00
		2993 A		PHE A	A	402	15.841	20.022	23.493	1.00
	ATOM 10.95	2994 A	CD2 C	PHE A	Ą	402	16.534	20.698	24.465	1.00
25	ATOM 15.85	2995 A		PHE .	A	402	18.725	22.896	27.641	1.00
	ATOM 16.80	2996 A	0	PHE .	A	402	18.356	24.021	27.952	1.00
30	ATOM 16.60		N N	ILE .	A	403	19.886	22.379	28.028	1.00
	ATOM 17.41	2998 A	CA C	ILE A	Ą	403	20.787	23.062	28.963	1.00

	ATOM 16.74		ILE	A	403	21.088	22.167	30.160	1.00
		3000 A	ILE	Α	403	19.802	21.886	30.944	1.00
5	ATOM 15.43	3001 A	ILE	A	403	19.946	20.733	31.931	1.00
	ATOM 17.20	3002 A	ILE	A	403	22.143	22.809	31.095	1.00
10	ATOM 17.62		ILE	A	403	22.064	23.395	28.240	1.00
		3004 A	ILE	A	403	22.812	22.520	27.854	1.00
	ATOM 18.39	3005 A	ASN	A	404	22.299	24.678	28.026	1.00
15	ATOM 19.61	3006 A	ASN	A	404	23.429	25.112	27.231	1.00
		3007 A	ASN	A	404	23.255	26.599	26.874	1.00
20	ATOM 26.59		ASN	A	404	24.297	27.071	25.913	1.00
	ATOM 32.24	3009 A	ASN	A	404	24.339	26.618	24.752	1.00
	ATOM 32.91	3010 A	ASN	A	404	25.177	27.980	26.381	1.00
25		3011 A	ASN	A	404	24.773	24.892	27.940	1.00
	ATOM 18.69	3012 A	ASN	A	404	25.769	24.575	27.296	1.00
30		3013 A	ALA	Α	405	24.779	25.020	29.262	1.00
	ATOM 19.42	3014 A	ALA	A	405	26.011	24.902	30.044	1.00

	ATOM 19.40			ALA	Α	405	26.450	26.317	30.582	1.00
	ATOM 19.12	3016 A		ALA	Α	405	25.787	23.934	31.217	1.00
5	ATOM 18.74				A	405	25.582	24.364	32.360	1.00
	ATOM 19.16	3018 A		PRO	A	406	25.782	22.632	30.936	1.00
10	ATOM 19.37			PRO	A	406	25.508	21.629	31.977	1.00
	ATOM 19.25			PRO	A	406	25.266	20.351	31.156	1.00
	ATOM 19.80	3021 A		PRO	A	406	26.120	20.546	29.977	1.00
15	ATOM 18.90			PRO	A	406	26.033	22.010	29.631	1.00
	ATOM 19.45	3023 A		PRO	Α	406	26.689	21.437	32.923	1.00
20	ATOM 19.95			PRO	Α	406	27.815	21.833	32.607	1.00
		3025 A		GLN	A	407	26.437	20.819	34.072	1.00
	ATOM 20.20		CA C	GLN	A	407	27.490	20.446	35.016	1.00
25	ATOM 21.02	3027 A	CB C	GLN	A	407	26.908	20.387	36.413	1.00
	ATOM 22.32	3028 A	CG C	GLN	A	407	26.155	21.620	36.805	1.00
30	ATOM 23.76	3029 A	CD C	GLN	A	407	25.122	21.323	37.849	1.00
	ATOM 21.20	3030 A	OE1 O	GLN	Α	407	25.320	20.443	38.713	1.00

	ATOM 22.99	3031 A		GLN	Α	407	24.016	22.040	37.789	1.00
	ATOM 20.27	3032		GLN	Α	407	28.062	19.075	34.675	1.00
5	ATOM 19.75	3033 A		GLN	A	407	27.392	18.232	34.057	1.00
		3034 A		SER	A	408	29.294	18.830	35.099	1.00
10	ATOM 20.08	3035 A		SER	A	408	29.869	17.491	35.033	1.00
	ATOM 20.55			SER	Α	408	31.393	17.538	35.212	1.00
	ATOM 19.34	3037 A		SER	A	408	32.042	18.067	34.072	1.00
15	ATOM 19.97			SER	A	408	29.269	16.615	36.120	1.00
	ATOM 20.96			SER	A	408	29.130	17.043	37.268	1.00
20	ATOM 19.80		N	GLY	A	409	28.980	15.362	35.775	1.00
	ATOM			GLY	A	409	28.447	14.392	36.715	1.00
	ATOM 19.28	3042 A	C C	GLY	A	409	27.216	13.697	36.160	1.00
25	ATOM 18.32	3043 A	0 0	GLY	A	409	27.026	13.646	34.940	1.00
	ATOM 18.72	3044 A	N N	THR	Α	410	26.350	13.224	37.058	1.00
30	ATOM 18.26	3045 A	CA C	THR	Α	410	25.226	12.396	36.678	1.00
	ATOM 17.98	3046 A	CB C	THR	Α	410	25.105	11.220	37.631	1.00

		3047 A		THR	Α	410	26.334	10.466	37.637	1.00
		3048 A		THR	Α	410	24.038	10.227	37.136	1.00
5	ATOM 18.19	3049 A		THR	Α	410	23.923	13.183	36.687	1.00
		3050 A		THR	A	410	23.510	13.735	37.718	1.00
10	ATOM 17.34			TYR	Α	411	23.274	13.241	35.524	1.00
	ATOM 16.46			TYR	A	411	21.942	13.783	35.430	1.00
	ATOM			TYR	Α	411	21.731	14.459	34.067	1.00
15		3054	CG	TYR	A	411	22.286	15.869	34.025	1.00
	ATOM		CD1	TYR	Α	411	21.458	16.953	34.156	1.00
20		3056	CE1	TYR	Α	411	21.956	18.231	34.131	1.00
20	.' ATOM		CZ	TYR	Α	411	23.319	18.438	33.994	1.00
	ATOM	3058	ОН	TYR	A	411	23.789	19.744	34.031	1.00
25	17.03 ATOM			TYR	Α	411	24.172	17.380	33.880	1.00
	ATOM	A 3060		TYR	A	411	23.660	16.099	33.889	1.00
	17.36 ATOM	A 3061	C C	TYR	Α	411	20.956	12.627	35.606	1.00
30	16.14	A	C	מעים	75	411	21.157	11 557	35.041	1.00
	ATOM 15.95	3062 A	0	IIK	А	411	21.13/	± ± > > /		00

	ATOM 15.50	3063 A		THR	Α	412	19.920	12.841	36.399	1.00
	ATOM 16.39			THR	A	412	18.760	11.959	36.418	1.00
5	ATOM 16.73	3065 A		THR	A	412	18.107	12.037	37.808	1.00
		3066 A		THR 2	A:	412	19.041	11.544	38.783	1.00
10				THR Z	A	412	16.877	11.115	37.946	1.00
	ATOM 16.26			THR	Α	412	17.764	12.397	35.344	1.00
		3069 A		THR	Α	412	17.404	13.568	35.286	1.00
15	ATOM 16.67		N N	VAL	Α	413	17.313	11.444	34.516	1.00
	ATOM 15.75			VAL .	A	413	16.342	11.672	33.452	1.00
20	ATOM 16.41	3072 A		VAL .	A	413	16.924	11.246	32.066	1.00
		3073 A		VAL 3	A	413	15.914	11.476	30.914	1.00
	ATOM 15.42	3074 A	CG2 C	VAL Z	A	413	18.240	11.946	31.773	1.00
25	ATOM 16.95	3075 A	C C	VAL	Α	413	15.134	10.811	33.791	1.00
	ATOM 18.21	3076 A	0 0	VAL .	A	413	15.232	9.574	33.667	1.00
30	ATOM 16.21	3077 A	N N	GLU	Α	414	14.040	11.439	34.256	1.00
	ATOM 17.01	3078 A	CA C	GLU .	A	414	12.803	10.774	34.736	1.00

	ATOM 16.06	3079 A	CB C	GLU	A	414		12.467	11.202	36.134	1.00
	ATOM 18.61			GLU	Α	414		11.518	10.244	36.767	1.00
5	ATOM 17.99	3081 A		GLU	A	414		11.626	10.318	38.265	1.00
	ATOM 20.38	3082 A		GLU	A	<b>4</b> 14		11.212	11.334	38.830	1.00
10		3083 A		GLU	A	414		12.198	9.404	38.810	1.00
	ATOM 16.05	3084 A		GLU	Α	414		11.715	11.142	33.729	1.00
		3085 A			A	414		11.428	12.301	33.528	1.00
15	ATOM 16.93			VAL	A	415	•	11.037	10.172	33.145	1.00
		3087 A		VAL	A	415		9.622	10.184	32.847	
20	ATOM 17.17	3088 A		VAL	Α	415		9.472	9.367	31.526	1.00
	ATOM 16.00	3089 A		VAL	Α	415		8.168	9.660	30.813	1.00
	ATOM 16.72	3090 A	CG2 C	VAL	A	415		10.652	9.660	30.622	1.00
25	ATOM 16.71	3091 A	C C	VAL	A	415		8.540	9.769	33.787	1.00
	ATOM 16.19	3092 A	0	VAL	A	415		8.463	8.634	34.185	1.00
30	ATOM 16.05	3093 A	N N	GLN	Α	416		7.684	10.736	34.077	1.00
	ATOM 16.43	3094 Á	CA C	GLN	Α	416		6.553	10.579	34.989	1.00

	ATOM 16.01	3095 A		GLN	A	416		6.519	11.747	35.981	1.00
		3096 A		GLN	Α	416		7.786	11.832	36.802	1.00
5	ATOM 17.22	3097 A		GLN	A	416		7.821	12.929	37.827	1.00
		3098 A		GLN	A	416		6.912	13.762	37.905	1.00
10		3099 A		GLN	A	416		8.933	12.972	38.601	1.00
		3100 A		GLN	A	416		5.232	10.504	34.235	1.00
		310 <sup>′</sup> 1 A		GLN	A	416		4.899	11.388	33.440	1.00
15		√3102 A		ALA	A	417		4.461	9.462	34.522	1.00
		3103 A		ALA	A	417		3.122	9.307	33.953	1.00
20	ATOM 18.16	3104 A		ALA	A	417		2.770	7.857	33.891	1.00
		3105 A		ALA	A	417		2.092	10.083	34.790	1.00
	ATOM 18.61	3106 A		ALA	Α	417	,	1.542	9.565	35.775	1.00
25	ATOM 19.27	3107 A	N N	TYR	A	418		1.859	11.338	34.437	1.00
	ATOM 20.10		CA C	TYR	A	418		0.944	12.153	35.234	1.00
30	ATOM 20.65	3109 A		TYR	A	418		0.985	13.618	34.803	1.00
	ATOM 23.36	3110 A	CG C	TYR	A	418		0.021	14.496	35.570	1.00

	ATOM 26.20	3111 A		TYR	A	418	0.255	14.818	36.908	1.00
	ATOM 29.96	3112 A		TYR	A	418	-0.645	15.610	37.625	1.00
5	ATOM 31.45			TYR	A	418	-1.772	16.099	36.990	1.00
	ATOM 34.45			TYR	A	418	-2.659	16.888	37.685	1.00
10	ATOM 29.32			TYR	A	418	-2.018	15.804	35.652	1.00
	ATOM 26.35	3116 A		TYR	A	418	-1.123	15.002	34.957	1.00
,		3117 A		TYR	Α	418	-0.477	11.623	35.158	1.00
15	ATOM 19.83			TYR	A	418	-1.142	11.445	36.190	1.00
	ATOM 19.39			ASN	A	419	-0.928	11.332	33.945	1.00
20	ATOM 19.40	3120 A		ASN	A	419	-2.284	10.855	33.708	1.00
	ATOM 20.03	3121 A		ASN	Α	419	-3.243	12.051	33.629	1.00
	ATOM 21.53	3122 A		ASN	A	419	-4.705	11.625	33.611	1.00
25	ATOM 23.42	3123 A	OD1 O	ASN	A	419	-5.094	10.758	34.354	1.00
	ATOM 22.67	3124 A	ND2 N	ASN	A	419	-5.493	12.212	32.727	1.00
30	ATOM 19.75	3125 A	C C	ASN	Α	419	-2.374	10.079	32.402	1.00
- <del>-</del>	ATOM 19.24			ASN	Α	419	-2.186	10.646	31.317	1.00

	ATOM		N	VAL .	A 420	-2.703	8.795	32.486	1.00
	19.24 ATOM	A 3128	N CA	<b>VAT.</b> 2	<u> 420</u>	-2.744	7 948	31 295	1 00
	18.57	A	C	VAL 7	1 420	-2.744	7.540	31.233	1.00
5	ATOM 18.55	3129 A	CB C	VAL A	A 420	-1.533	6.986	31.288	1.00
	ATOM 17.15	3130 A	CG1 C	VAL A	420	-1.504	6.086	30.040	1.00
10	ATOM 20.43	3131 A	CG2 C	VAL A	420	-0.196	7.799	31.402	1.00
	ATOM 18.55	3132 A	C C	VAL A	A 420	-4.067	7.165	31.234	1.00
	ATOM 18.55	3133 A	0 .	VAL A	A 420	-4.109	5.996	31.606	1.00
15	ATOM 18.79	3134 A	N N	PRO A	A 421	-5.132	7.816	30.776	1.00
	ATOM 19.54	3135 A	CA C	PRO A	421	-6.444	7.169	30.635	1.00
20	ATOM 19.65	3136 A	CB C	PRO A	421	-7.397	8.324	30.288	1.00
	ATOM 19.70	3137 A	CG C	PRO A	421	-6.540	9.394	29.746	1.00
	ATOM 18.68		CD C	PRO A	421	-5.175	9.239	30.396	1.00
25 ·	ATOM 19.68	3139 A	C C	PRO A	421	-6.507	6.141	29.530	1.00
	ATOM 20.15		0 0	PRO A	421	-7.411	5.318	29.565	1.00
30	ATOM 19.04	3141 A	N N		. 422	-5.592	6.178	28.566	1.00
	ATOM 18.85	3142 A	CA C	VAL A	422	-5.594	5.180	27.505	1.00

	ATOM 18.35	3143 A		VAL	Α	422	-5.990	5.781	26.146	1.00
		3144 A		VAL	A	422	-6.200	4.653	25.091	1.00
5	ATOM 18.28	3145 A		VAL	A	422	-7.264	6.616	26.285	1.00
	_	3146 A		VAL	A	422	-4.226	4.509	27.448	1.00
10	ATOM 18.38			VAL	A	422	-3.435	4.713	26.505	1.00
		3148 A		GLY	A	423	-3.957	3.707	28.480	1.00
		3149 · A		GLY	A	423	2.642	3.150	28.702	1.00
15		3150 A		GLY	A	423	-2.510	1.665	28.496	1.00
		3151 A		GLY	A	423	-3.464	0.954	28.162	1.00
20	ATOM 19.10	3152 A		PRO	A	424	-1.307	1.174	28.695	1.00
,	ATOM 17.55	3153 A		PRO	A	424	-0.142	1.999	29.040	1.00
	ATOM 18.01		CB C	PRO	A	424	0.876	0.969	29.467	1.00
25	ATOM 19.87	3155 A	CG Č	PRO	A	424	0.510	-0.258	28.696	1.00
	ATOM 19.26	3156 A	CD C	PRO	A	424	-0.988	-0.267	28.649	1.00
30	ATOM 16.87	3157 A	C C	PRO	A	424	0.396	2.842	27.899	1.00
	ATOM 17.20	3158 · A	0 0	PRO	A	424	. 0.038	2.660	26.733	1.00

	ATOM 15.38			A	425	1.248	3.798	28.239	1.00
	ATOM 14.36		GLN	A	425	1.848	4.678	27.240	1.00
5	ATOM 14.88	3161 A	GLN	Α	425	1.507	6.140	27.559	1.00
	ATOM 14.70	3162 A	GLN	Α	425	2.070	7.202	26.576	1.00
10	ATOM 16.71		GLN	Α	425	1.512	7.043	25.180	1.00
	ATOM 15.27		GLN	A	425	0.321	7.321	24.956	1.00
	ATOM 11.93	3165 A	GLN	A	425	2.349	6.580	24.235	1.00
15	ATOM 13.10	3166 A	GLN	A	425	3.341	4.470	27.252	1.00
	ATOM 12.18		GLN	A	425	3.987	4.662	28.283	1.00
20	ATOM 12.88	3168 A	THR	A	426	3.887	4.036	26.112	1.00
	ATOM 12.90	3169 A	THR	Α	426	5.320	4.008	25.913	1.00
	ATOM 12.37		THR	A	426	5.737	2.949	24.890	1.00
25	ATOM 12.70		THR	Α	426	5.134	3.254	23.626	1.00
	ATOM 13.56	3172 A	THR	Α	426	5.232	1.573	25.283	1.00
30	ATOM 13.16		THR	Α	426	5.796	5.370	25.413	1.00
	ATOM 14.38	3174 A	THR	Α	426	4.986	6.223	25.037	1.00

	ATOM 12.86	3175 A		A	427	7.115	5.551	25.401	1.00
	ATOM 12.44		PHE	A	427	7.741	6.823	25.036	1.00
5		3177 A	PHE	Α	427	7.802	7.778	26.240	1.00
		3178 A	PHE	Α	427	8.612	7.235	27.366	1.00
10		3179 A	PHE	Α	427	9.988	7.361	27.365	1.00
	ATOM 15.74		PHE	A	427	10.768	6.801	28.381	1.00
		3181 A	PHE	A	427	10.161	6.102	29.408	1.00
15	ATOM 16.39	3182 A	PHE	Α	427	8.766	5.987	29.427	1.00
		3183 A	PHE	Α	427	8.000	6.538	28.407	1.00
20		3184 A	PHE	A	427	9.149	6.532	24.549	1.00
		3185 A	PHE	Α	427	9.694	5.444	24.807	1.00
		3186 A	SER	Α	428	9.721	7.523	23.867	1.00
25	ATOM 11.99	3187 A	SER	Α	428	11.116	7.528	23.480	1.00
		3188 A	SER	Α	428	11.292	7.463	21.965	1.00
30	ATOM 12.32	3189 A	SER	Α	428	10.837	6.219	21.442	1.00
		3190 A	SER	A	428	11.804	8.776	24.031	1.00

	ATOM	3191	0	SER	Α	428	11.174	9.829	24.263	1.00
	11.91	A	0							
	ATOM 12.35	3192 A			A	429	13.103	8.620	24.278	1.00
5	ATOM 12.57	3193 A		LEU	A	429	13.950	9.712	24.714	1.00
		3194 A		LEU	Α	429	14.508	9.476	26.135	1.00
10		3195 A		LEU	A	429	13.542	9.648	27.296	1.00
		3196 A		LEU	Α	429	14.046	8.907	28.520	1.00
	ATOM 15.64	3197 A		LEU	Α	429	13.348	11.110	27.609	1.00
15		3198 A		LEU	Α	429	15.098	9.756	23.768	1.00
		3199 A		LEU	Α	429	15.593	8.707	23.372	1.00
20	ATOM 11.55	3200 A		ALA	Α	430	15.532	10.957	23.405	1.00
		3201 A		ALA	Α	430	16.805	11.139	22.699	1.00
	ATOM 12.63		CB C	ALA	Α	430	16.581	11.528	21.235	1.00
25		3203 A		ALA	Α	430	17.613	12.215	23.404	1.00
	ATOM 12.14	3204 A		ALA	A	430	17.072	13.256	23.776	1.00
30		3205 A		ILE	A	431	18.907	11.943	23.584	1.00
	ATOM 13.32	3206 A		ILE	Α	431	19.813	12.835	24.287	1.00

	ATOM 13.00	3207 A		ILE A	431		20.325	12.179	25.593	1.00
J	ATOM 14.30	3208 A	CG1 C	ILE A	431		19.175	11.882	26.542	1.00
5	ATOM 16.21	3209 A		ILE A	431		19.575	11.061	27.776	1.00
	ATOM 14.86	3210 A		ILE A	431		21.292	13.123	26.288	1.00
10	ATOM 12.92	3211 A		ILE A	431		21.005	13.176	23.392	1.00
		3212 A		ILE A	. 431		21.728	12.288	22.937	1.00
	ATOM 13.80	3213 A		VAL A	432		21.192	14.464	23.134	1.00
15	ATOM 15.20	3214 A	CA C	VAL A	432		22.387	14.966	22.483	1.00
	ATOM 15.89	3215 A		VAL A	432	,	22.028	15.996	21.387	1.00
20	ATOM 15.25	3216 A		VAL A	432		23.293	16.591	20.809	1.00
	ATOM 15.39	3217 A		VAL A	432		21.167	15.361	20.293	1.00
	ATOM 16.38			VAL A	432		23.346	15.634	23.498	1.00
25	ATOM 16.49			VAL A	432		22.923	16.472	24.298	1.00
	ATOM 17.45			HIS A		t	24.633	15.257	23.458	1.00
30	ATOM 18.55			HIS A	433		25.669	15.872	24.306	1.00
	ATOM 19.21	3222 A		HIS A	433		25.637	15.240	25.711	1.00

	ATOM 19.32	3223 A			A	433	26.553	15.885	26.707	1.00
	ATOM 18.22				A	433	26.497	17.233	27.015	1.00
5	ATOM 18.90	3225 A		HIS	A	433	27.378	17.497	27.969	1.00
	ATOM 16.51			HIS	A	433	27.999	16.380	28.289	1.00
10		3227 A		HIS	A	433	27.502	15.353	27.513	1.00
	ATOM 19.74			HIS	A	433	27.031	15.627	23.684	1.00
	ATOM 21.68	3229 A		HIS	A	433	27.664	16.546	23.133	1.00
15	ATOM 19.29	3230 A		HIS	Α	433	27.463	14.480	23.735	1.00
	TER	3230	H	HIS A	43	33				
	HETATM 16.92			CA	Α	601	15.429	35.876	3.369	1.00
20	HETATM 13.45			CA	A	602	3.346	16.597	30.346	1.00
	HETATM 17.30				A	603	9.615	28.353	34.891	1.00
25	ATOM 49.01	3234 B	N N	ASP	В	16	3.955	53.303	-10.201	1.00
	ATOM 49.32	3235 B	CA C	ASP	В	16	4.171	51.870	-9.771	1.00
	ATOM 49.78	3236 B	CB C	ASP	В	16	5.553	51.425	-10.270	1.00
30	ATOM 52.12	3237 B	CG C	ASP	В	16	6.176	52.438	-11.248	1.00
	ATOM 54.86	3238 B		ASP	В	16	5.667	52.549	-12.399	1.00

	ATOM 52.51	3239 B	OD2 O	ASP	В	16	7.151	53.181	-10.957	1.00
	ATOM 48.45	3240 B	C C	ASP	В	16	4.009	51.690	-8.232	1.00
5	ATOM 47.87	3241 B		ASP	В	16	4.793	50.996	-7.567	1.00
	ATOM 47.87	3242 B	N N	ARG	В	17	2.959	52.301	-7.687	1.00
10	ATOM 47.30	3243 B	CA C	ARG	В	17	2.863	52.592	-6.247	1.00
	ATOM 46.77		CB C	ARG	В	17	2.430	54.064	-6.059	1.00
	ATOM 44.50	3245 B		ARG	В	17	3.107	55.055	-7.028	1.00
15	ATOM 39.98	3246 B	CD C	ARG	В	17	2.860	56.528	-6.691	1.00
	ATOM 33.05	3247 B		ARG	В	17	3.266	56.891	-5.335	1.00
20	ATOM 29.36	3248 B		ARG	В	17	4.483	57.334	-5.001	1.00
•	ATOM 28.07		NH1 N	ARG	В	17	5.440	57.459	-5.915	1.00
	ATOM 24.57	3250 B	NH2 N	ARG	B	17	4.752	57.650	-3.740	1.00
25	ATOM 48.01	3251 B	C C	ARG	В	17	1.917	51.699	-5.415	1.00
	ATOM 47.42	3252 B	0 0	ARG	В	17	1.463	52.120	-4.342	1.00
30	ATOM 48.51	3253 B	N N	HIS	В	18	1.616	50.486	-5.885	1.00
	ATOM 48.98	3254 B	CA C	HIS	В	18	0.770	49.573	-5.108	1.00

	ATOM 49.29	3255 B	CB C	HIS	В	18	0.515	48.266	-5.875	1.00
	ATOM 50.05	3256 B	CG C	HIS	В	18	-0.510	48.388	-6.961	1.00
5	ATOM 51.24	3257 B	ND1 N	HIS	В	18	-0.195	48.803	-8.238	1.00
	ATOM 51.27	3258 B	CE1 C	HIS	В	18	-1.291	48.814	-8.979	1.00
10	ATOM 50.69	3259 B		HIS	В	18	-2.305	48.419	-8.228	1.00
	ATOM 50.64	3260 B	CD2 C	HIS	В	18	-1.844	48.147	-6.962	1.00
	ATOM 49.16	3261 B		HIS	В	18	1.429	49.229	-3.770	1.00
15	ATOM 49.03	3262 B	0 0	HIS	В	18	2.598	48.822	-3.738	1.00
	ATOM 49.15	3263 B		ASN	В	19	0.690	49.386	-2.667	1.00
20	ATOM 49.11	3264 B		ASN	В	19	1.167	48.868	-1.384	1.00
	ATOM 49.60			ASN	В	19	0.276	49.313	-0.205	1.00
	ATOM 51.24	3266 B	CG C	ASN	В	19	0.951	49.099	1.176	1.00
25	ATOM 53.59	3267 B	OD1 O	ASN	В	19	0.415	48.415	2.058	1.00
	ATOM 54.56	3268 B	ND2 N	ASN	В	19	2.123	49.705	1.363	1.00
30	ATOM 48.22	3269 B	C C	ASN	<b>B</b> :	19	1.241	47.332	-1.459	1.00
	ATOM 47.43	3270 B	0 0	ASN	В	19	0.443	46.685	-2.138	1.00

	ATOM 47.20	3271 B	N N	LEU	В	20	2.221	46.772	-0.762	1.00
	ATOM 46.38	3272 B	CA C	LEU	В	20	2.393	45.333	-0.689	1.00
5	ATOM 46.97	3273 B	CB C	LEU	В	20	3.743	45.000	-0.055	1.00
	ATOM 48.40	3274 B	CG C	LEU	В	20	4.896	45.800	-0.684	1.00
10	ATOM 49.54	3275 B	CD1 C	LEU	В	20	6.201	45.666	0.117	1.00
	ATOM 48.69	3276 B	CD2 C	LEU	В	20	5.076	45.391	-2.158	1.00
	ATOM 44.75	3277 B	C C	LEU	В	20	1.235	44.792	0.141	1.00
15	ATOM 45.26	3278 B	0 0	LEU	В	20	1.113	45.092	1.342	1.00
	ATOM 41.97	3279 B	N N	LYS	В	21	0.338	44.073	-0.523	1.00
20	ATOM 39.98	3280 B	CA C	LYS	В	21	-0.740	43.395	0.170	1.00
	ATOM 40.54	3281 B	CB C	LYS	В	21	-2.088	44.025	-0.183	1.00
	ATOM 41.63	3282 B	CG C	LYS	В	21	-3.225	43.550	0.700	1.00
25	ATOM 43.44	3283 B	CD C	LYS	В	21	-4.257	44.620	0.878	1.00
	ATOM 44.82	3284 B	CE C	LYS	В	21	-5.391	44.131	1.718	1.00
30	ATOM 47.17	3285 B	NZ N	LYS	В	21	-4.992	44.004	3.147	1.00
	ATOM 37.09	3286 B	C C	LYS	В	21	-0.710	41.917	-0.214	1.00

	ATOM 35.80	3287 B	O	S B	21	-0.679	41.588	-1.395	1.00
	ATOM 33.91	3288 B	N TH	IR B	22	-0.685	41.045	0.796	1.00
5	ATOM 31.44	3289 B	CA TH C	R B	22	-0.642	39.592	0.593	1.00
	ATOM 31.70	3290 B	CB TH C	RВ	22	0.734	39.046	1.030	1.00
10	ATOM 31.47	3291 B	OG1 TH	RВ	22	1.002	39.436	2.387	1.00
	ATOM 31.30	3292 B	CG2 TH	R B	22	1.857	39.681	0.211	1.00
		3293 B	C TH	R B	22	-1.739	38.843	1.342	1.00
15	ATOM 28.17	3294 B	O TH O	R B	22	-1.830	37.617	1.246	1.00
		3295 B	N GL	UВ	23	-2.542	39.576	2.107	1.00
20	ATOM 27.22	3296 B	CA GL	UB	23	-3.672	39.011	2.828	1.00
	ATOM 27.51	3297 B	CB BGL	JВ	23	-3.280	38.728	4.282	0.50
	ATOM 27.17	3298 B	CB AGLI C	JВ	23	-3.287	38.646	4.277	0,50
25	ATOM 29.10	3299 B	CG BGLI	JВ	23	-2.826	37.304	4.512	0.50
	ATOM 27.55	3300 B	CG AGL	JВ	23	-3.050	39.822	5.223	0.50
30		3301 , B	CD BGL	JВ	23	-2.236	37.062	5.891	0.50
	ATOM 28.07	3302 B	CD AGLU	JВ	23	-3.020	39.396	6.689	0.50

	ATOM 32.02	3303 B	OE1E O	BGLU	В	23	-1.959	38.040	6.614	0.50
	ATOM 28.41	3304 B		AGLU	В	23	-2.853	38.186	6.954	0.50
5	ATOM 31.16	3305 B		BGLU	В	23	-2.054	35.879	6.241	0.50
	ATOM 28.60	3306 B		AGLU	В	23	-3.182	40.264	7.579	0.50
10	ATOM 25.94		C C	GLU	В	23	-4.842	39.988	2.799	1.00
	ATOM 25.17		0 0	GLU	В	23	-4.631	41.199	2.805	1.00
	ATOM 24.57		N N	TRP	В	24	-6.065	39.462	2.765	1.00
15	ATOM 23.89	3310 B	CA C	TRP	В	24	-7.264	40.300	2.708	1.00
	ATOM 23.59	3311 B		TRP	В	24	-7.910	40.174	1.304	1.00
20	ATOM 21.71	3312 B		TRP	В	24	-7.105	40.786	0.245	1.00
	ATOM 21.02		CD1 C	TRP	В	24	-7.232	42.050	-0.239	1.00
	ATOM 18.62	3314 B	NE1 N	TRP	В	24	-6.293	42.276	-1.211	1.00
25	ATOM 19.02	3315 B	CE2 C	TRP	В	24	-5.544	41.148	-1.396	1.00
	ATOM 20.72	3316 B	CD2 C	TRP	В	24	-6.006	40.190	-0.480	1.00
30	ATOM 19.49	3317 B	CE3 C	TRP	В	24	-5.387	38.941	-0.454	1.00
	ATOM 20.25	3318 ·	CZ3 C	TRP	В	24	-4.326	38.694	-1.313	1.00

	ATOM 21.63	3319 B	CH2 C		В	24	-3.883	39.662	-2.207	1.00
	ATOM 22.09	3320 B	CZ2 C		В	24	-4.477	40.911	-2.257	1.00
5	ATOM 23.91	3321 B	C C		В	24	-8.294	39.948	3.789	1.00
	ATOM 22.74	3322 B	0 0	TRP	В	24	-9.369	39.456	3.467	1.00
10	ATOM 24.64	3323 B	N N		В	25	-7.986	40.196	5.070	1.00
	ATOM 25.12	3324 B		PRO	В	25	-8.918	39.850	6.161	1.00
	ATOM 25.87	3325 B	CB C	PRO	В	25	-8.176	40.312	7.448	1.00
15	ATOM 26.08	3326 B	CG C	PRO	В	25	-7.011	41.163	7.002	1.00
	ATOM 25.49	3327 B	CD C	PRO	В	25	-6.737	40.807	5.562	1.00
20	ATOM 25.18	3328 B	C C	PRO	В	25	-10.307	40.520	6.029	1.00
	ATOM 24.94	3329 B	0 0	PRO	В	25	-11.310	39.978	6.469	1.00
	ATOM 25.43	3330 B	N N	GLU	B	26	-10.350	41.668	5.364	1.00
25	ATOM 25.93	3331 B	CA C	GLU	В	26	-11.581	42.416	5.141	1.00
	ATOM 26.70	3332 B	CB C	GLU	В	26	-11.243	43.829	4.627	1.00
30	ATOM 28.62	3333 B	CG C	GLU	В	26	-10.690	43.922	3.189	1.00
	ATOM 29.61	3334 B	CD C	GLU	В	26	-9.169	43.775	3.077	1.00

	ATOM 28.68	3335 B		GLU	В	26	-8.535	43.174	3.985	1.00
	ATOM 31.71	3336 B		GLU	В	26	-8.608	44.252	2.057	1.00
5	ATOM 25.60	3337 B		GLU	В	26	-12.571	41.705	4.193	1.00
	ATOM 24.75	3338 B	0 0	GLU	В	26	-13.746	42.060	4.139	1.00
10	ATOM 24.52		N N	LEU	В	27	-12.119	40.672	3.483	1.00
	ATOM 23.54	3340 B		LEU	В	27	-12.957	40.024	2,483	1.00
	ATOM 23.84	3341 B	CB C	LEU	В	27	-12.104	39.593	1.287	1.00
15	ATOM 23.08	3342 B	CG <sub>.</sub> C	LEU	В	27	-11.506	40.722	0.430	1.00
	ATOM 22.31	3343 B		LEU	В	27	-10.702	40.165	-0.732	1.00
20	ATOM 23.37	3344 B		LEU	В	27	-12.603	41.624	-0.097	1.00
	ATOM 23.75	3345 B		LEU	В	27	-13.716	38.829	3.042	1.00
	ATOM 23.33	3346 B	0 0	LEU	В	27	-14.504	38.205	2.334	1.00
25	ATOM 23.89	3347 B	N N	VAL	В	28	-13.490	38.504	4.312	1.00
	ATOM 24.64	3348 B	CA C	VAL	В	28	-14.143	37.357	4.918	1.00
30	ATOM 24.78	3349 B	CB C	VAL	В	28	-13.571	37.050	6.359	1.00
	ATOM 25.39	3350 B	CG1 C	VAL	В	28	-14.359	35.963	7.027	1.00

	ATOM 25.78	3351 B	CG2 C	VAL	В	28	-12.099	36.634	6.272	1.00
	ATOM 24.75	3352 B	C C	VAL	В	28	-15.612	37.694	4.992	1.00
5	ATOM 25.68	3353 B	0	VAL	В	28	-15.952	38.791	5.424	1.00
	ATOM 24.86	3354 B	N N	GLY	В	29	-16.468	36.797	4.516	1.00
10	ATOM 24.80	3355 B	CA C	GLY	В	29	-17.916	37.000	4.539	1.00
	ATOM 25.07	3356 B	C C	GLY	В	29	-18.493	37.638	3.274	1.00
	ATOM 25.27	3357 B	0 0	GLY	В	29	-19.692	37.598	3.061	1.00
15	ATOM 25.21	3358 B	N N	LYS	В	30	-17.630	38.203	2.429	1.00
	ATOM 24.62	3359 B	CA C	LYS	В	30	-18.025	38.782	1.146	1.00
20	ATOM 25.65	3360 B	CB C	LYS	В	30	-16.952	39.780	0.679	1.00
	ATOM 28.42	3361 B	CG C	LYS	В	30	-16.716	40.964	1.606	1.00
	ATOM 34.26	3362 B	CD C	LYS	В	30	-16.577	42.245	0.785	1.00
25	ATOM 35.92	3363 B	CE C	LYS	В	30	-16.462	43.527	1.631	1.00
	ATOM 37.72	3364 B	NZ N	LYS	В	30	-15.996	43.273	3.011	1.00
30	ATOM 23.30	3365 B	C C	LYS	В	30	-18.188	37.728	0.065	1.00
	ATOM 22.29	3366 B	0 0	LYS	В	30	-17.670	36.623	0.166	1.00

	ATOM 21.94	3367 B	N SER B N	31	-18.884	38.089	-1.001	1.00
	ATOM 20.89	3368 B	CA SER B	31	-19.036	37.204	-2.145	1.00
5	ATOM 21.21	3369 B		31	-20.046	37.776	-3.143	1.00
	ATOM 20.40	3370 B		31	-19.519	38.912	-3.815	1.00
10	ATOM 19.88	3371 B	C SER B	31	-17.726	37.017	-2.865	1.00
	ATOM 18.67	3372 B	O SER B	31	-16.828	37.843	-2.800	1.00
	ATOM 20.34	3373 B	N VAL B	32	-17.649	35.920	-3.588	1.00
15	ATOM 20.89	3374 B	CA VAL B	32	-16.487	35.617	-4.393	1.00
	ATOM 20.94	3375 B	CB BVAL B	32	-16.717	34.256	-5.141	0.50
20	ATOM 21.07	3376 B	CB AVAL B	32	-16.555	34.234	-5.043	0.50
	ATOM 20.85	3377 B	CG1BVAL B	32	-16.023	34.221	-6.524	0.50
	ATOM 20.79	3378 B	CG1AVAL B	32	-17.648	34.180	-6.069	0.50
25	ATOM 20.73	3379 B	CG2BVAL B	32	-16.276	33.087	-4.281	0.50
	ATOM 21.36	3380 B	CG2AVAL B	32	-15.193	33.903	-5.657	0.50
30	ATOM 20.83	3381 B	C VAL B	32	-16.238	36.732	-5.431	1.00
	ATOM 20.37	3382 B	O VAL B	32	-15.100	37.105	-5.681	1.00

	ATOM 21.19	3383 B	N N	GLU I	3 3 3 3	-17.316	37.263	-6.011	1.00
	ATOM 21.20	3384 B	CA C	GLU E	3 33	-17.205	38.264	-7.072	1.00
5	ATOM 21.59	3385 B	CB C		3 33	-18.553	38.478	-7.767	1.00
	ATOM 24.67	3386 B	CG C	GLU E	3 33	-19.045	37.271	-8.543	1.00
10	ATOM 29.01	3387 B	CD C	GLU E	3 33	-19.799	36.219	-7.708	1.00
	ATOM 36.54	3388 B	OE1 O	GLU B	33	-20.001	35.123	-8.275	1.00
	ATOM 27.78	3389 B	OE2 O	GLU B	33	-20.187	36.437	-6.517	1.00
15	ATOM 20.62	3390 B	C	GLU B	3 3 3	-16.688	39.571	-6.497	1.00
	ATOM 20.20	3391 B	0	GLU B	33	-15.885	40.255	-7.130	1.00
20	ATOM 20.61	3392 B	N N	GLU B	34	-17.124	39.910	-5.283	1.00
	ATOM 20.97	3393 B	CA C	GLU B	34	-16.627	41.131	-4.634	1.00
	ATOM 21.10	3394 B	CB C	GLU B	34	-17.456	41.533	-3.407	1.00
25	ATOM 25.82	3395 B	CG C	GLU B	34	-18.778	42.224	-3.722	1.00
	ATOM 31.16	3396 B	CD C	GLU B	34	-18.615	43.546	-4.481	1.00
30	ATOM 32.84	3397 B	OE1 O	GLU B	34	-17.968	44.484	-3.932	1.00
	ATOM 33.71	3398 B	OE2 O	GLU B	34	-19.135	43.645	-5.626	1.00

	ATOM 19.67	3399 B	C C	GLU B	34	-15.156	40.951	-4.257	1.00
	ATOM 18.91		0	GLU B	34	-14.340	41.858	-4.438	1.00
5	ATOM 19.75			ALA B	35	-14.809	39.775	-3.765	1.00
	ATOM 19.10	3402 B	CA C	ALA B	35	-13.414	39.485	-3.401	1.00
10	ATOM 19.66		CB C	ALA B	35	-13.311	38.127	-2.749	1.00
	ATOM 18.90		C C	ALA B	35	-12.457	39.581	-4.582	1.00
	ATOM 18.82	3405 B		ALA B	35	-11.387	40.183	-4.470	1.00
15	ATOM 18.68		N N	LYS B	36	-12.839	38.993	-5.716	1.00
	ATOM 18.17	3407 B	CA C	LYS B	36 .	-11.991	38.978	-6.894	1.00
20	ATOM 18.44	3408 B		LYS B	36	-12.659	38.220	-8.063	1.00
	ATOM 19.56	3409 B		LYS B	36	-12.714	36.693	-7.928	1.00
•	ATOM 20.72	3410 B	CD C	LYS B	36	-13.304	36.026	-9.159	1.00
25	ATOM 22.32	3411 B	CE C	LYS B	36	-13.194	34.496	-9.136	1.00
	ATOM 20.54	3412 B	NZ N	LYS B	36	-13.963	33.865	-10.274	1.00
30	ATOM 17.67	3413 B	C C	LYS B	36	-11.648	40.406	-7.316	1.00
	ATOM 17.81	3414 B	0 0	LYS B	36	-10.500	40.694	-7.681	1.00

	ATOM 17.52	3415 B	Ñ N		В	37	-12.614	41.316	-7.254	1.00
	ATOM 17.89	3416 B	CA C		В	37	-12.345	42.667	-7.746	1.00
5	ATOM 17.35	3417 B	CB C		В	37	-13.621	43.519	-7.870	1.00
	ATOM 17.43	3418 B	CG C	LYS	В	37	-14.544	43.165	-9.036	1.00
10	ATOM 15.06	3419 B	CD C	LYS		37	-15.847	44.074	-9.064	1.00
	ATOM 16.48	3420 B	CE C	LYS	В	37	-16.801	43.812	-7.921	1.00
	ATOM 15.66	3421 B	NZ N	LYS	В	37	-18.031	44.685	-7.989	1.00
15	ATOM 18.04	3422 B	C C	LYS	В	37	-11.333	43.372	-6.852	1.00
	ATOM 18.33	3423 B	0	LYS	В	37	-10.499	44126	-7.354	1.00
20	ATOM 17.93	3424 B	N N	VAL	В	38	-11.436	43.174	-5.535	1.00
	ATOM 18.53	3425 B	CA C	VAL	В	38	-10.525	43.824	-4.595	1.00
	ATOM 19.32	3426 B	CB C	VAL	В	38	-11.024	43.636	-3.136	1.00
25	ATOM 21.52	3427 B	CG1 C	VAL	В	38	-9.975	44.055	-2.128	1.00
	ATOM 20.73	3428 B	CG2 C	VAL	В	38	-12.310	44.445	-2.919	1.00
30	ATOM 18.91	3429 B	C C	VAL	В	38	-9.122	43.270	-4.742	1.00
	ATOM 17.79	3430 B	0 0	VAL	В.	38	-8.135	44.013	-4.797	1.00

	ATOM 19.11	3431 B	N N	ILE	В	39	-9.033	41.947	-4.830	1.00
	ATOM 19.64	3432 B	CA C	ILE	В	39	-7.747	41.304	-5.009	1.00
5	ATOM 19.43	3433 B	CB C	ILE	В	39	-7.919	39.764	-4.973	1.00
	ATOM 20.37	3434 B	CG1 C	ILE	В	39	-8.288	39.324	-3.573	1.00
10	ATOM 21.36	3435 B	CD1 C	ILE	В	39	-8.994	37.995	-3.564	1.00
	ATOM 19.76	3436 B	CG2 C	ILE	В	39	-6.657	39.024	-5.470	1.00
	ATOM 19.71	3437 B	C C	ILE	В	39	-7.077	41.759	-6.287	1.00
15	ATOM 19.70	3438 B	0 0	ILE	В	39	-5.877	42.087	-6.266	1.00
	ATOM 19.22	3439 B	N N	LEU	В	40	-7.816	41.785	-7.404	1.00
20	ATOM 19.62	3440 B	CA C	LEU	В	40	-7.205	42.231	-8.664	1.00
	ATOM 19.18	3441 B	CB C	LEU	В	40	-8.100	41.927	-9.888	1.00
	ATOM 20.23	3442 B	CG C	LEU	В	40	-8.145	40.416	-10.190	1.00
25	ATOM 19.43	3443 B	CD1 C	LEU	В	40	-9.235	40.047	-11.123	1.00
	ATOM 21.26	3444 B	CD2 C	LEU	В	40	-6.799	39.947	-10.725	1.00
30	ATOM 19.20	3445 B	C C	LEU	В	40	-6.840	43.716	-8.608	1.00
	ATOM 19.48	3446 B	0 0	LEU	В	40	-5.939	44.144	-9.300	1.00

	ATOM 19.70	3447 B	N N	GLN	В	41	-7.553	44.494	-7.803	1.00
	ATOM 20.69	3448 B	CA C	GLN	В	41	-7.216	45.914	-7.622	1.00
5	ATOM 20.30	3449 B	CB C	GLN	В	41	-8.286	46.641	-6.813	1.00
	ATOM 20.90	3450 B	CG C	GLN	В	41	-8.068	48.173	-6.731	1.00
10	ATOM 21.54	3451 B	CD C	GLN	В	41	-8.159	48.842	-8.083	1.00
	ATOM 23.88	3452 B	OE1 O	GLN	В	41	-9.070	48.529	-8.858	1.00
	ATOM 20.95	3453 B	NE2 N	GLN	В	41	-7.224	49.762	-8.384	1.00
15	ATOM 22.10	3454 B	C C	GLN	В	41	-5.880	46.050	-6.906	1.00
	ATOM 22.64	3455 B	0 0	GLN	В	41	-5.105	46.941	-7.213	1.00
20	ATOM 22.70	3456 B	N N	ASP	В	42	-5.625	45.149	-5.955	1.00
	ATOM 23.28	3457 B	CA C	ASP	В	42	-4.396	45.178	-5.161	1.00
	ATOM 22.77	3458 B	CB C	ASP	В	42	-4.654	44.531	-3.800	1.00
25	ATOM 24.12	3459 B	CG C	ASP	В	42	-5.531	45.369	-2.928	1.00
	ATOM 27.20	3460 B	OD1 O	ASP	В	42	-5.619	46.599	-3.174	1.00
30	ATOM 25.78	3461 B	OD2 O	ASP	В	42	-6.206	44.899	-1.991	1.00
	ATOM 23.19	3462 B	C C	ASP	В	42	-3.273	44.438	-5.859	1.00

	ATOM 24.27	3463 B	0 0	ASP	В	42	-2.103	44.761	-5.700	1.00
	ATOM 22.96	3464 B	N N	LYS	В	43	-3.629	43.444	-6.655	1.00
5	ATOM 23.10	3465 B	CA C	LYS	В	43	-2.634	42.541	-7.203	1.00
	ATOM 23.07	3466 B	CB C	LYS	В	43	-2.508	41.291	-6.299	1.00
10	ATOM 23.16	3467 B	CG C	LYS	В	43	-1.376	40.306	-6.701	1.00
	ATOM 24.15	3468 B		LYS	В	43	-1.348	39.100	-5.750	1.00
	ATOM 25.40	3469 B	CE C	LYS	В	43	-0.391	37.996	-6.217	1.00
15	ATOM 25.72	3470 B	NZ N	LYS	В	43	1.031	38.403	-6.170	1.00
	ATOM 23.00	3471 B	C C	LYS	В	43	-3.067	42.157	-8.593	1.00
20	ATOM 22. 17	3472 B	0 0	LYS	В	43	-3.672	41.107	-8.782	1.00
	ATOM 24.07		N N	PRO	В	44	-2.772	43.010	-9.571	1.00
	ATOM 24.35	3474 B	CA C	PRO	В	44	-3.282	42.826	-10.948	1.00
25	ATOM 24.65	3475 B	CB C	PRO	В	44	-2.632	43.985	-11.735	1.00
	ATOM 25.50	3476 B	CG C	PRO	В	44	-2.197	44.997	-10.702	1.00
30	ATOM 24.73	3477 B	CD C	PRO	В	44	-1.960	44.238	-9.415	1.00
	ATOM 24.65	3478 B	C C	PRO	В	44	-2.929	41.486	-11.583	1.00

	ATOM 25.49	3479 B	0	PRO B	44	-3.680	40.967	-12.409	1.00
	ATOM 25.20	3480 B	N N	GLU B	45	-1.778	40.935	-11.206	1.00
5	ATOM 25.70	3481 B	CA C	GLU B	45	-1.310	39.651	-11.725	1.00
	ATOM 26.83	3482 B	CB C	GLU B	45	0.226	39.599	-11.602	1.00
10	ATOM 28.74	3483 B	CG C	GLU B	45	0.764	39.243	-10.206	1.00
	ATOM 32.92	3484 B	CD C	GLU B	45	0.925	40.423	-9.262	1.00
	ATOM 34.10	3485 B	OE1 O	GLU B	45	1.667	40.252	-8.253	1.00
15	ATOM 33.16	3486 B	OE2 O	GLU B	45	0.316	41.511	-9.488	1.00
	ATOM 25.32	3487 B	C C	GLU B	45	-1.945	38.404	-11.048	1.00
20	ATOM 25.52	3488 B	0 0	GLU B	45	-1.679	37.270	-11.452	1.00
	ATOM 24.59	3489 B	N N	ALA B	46	-2.788	38.593	-10.034	1.00
	ATOM 23.90	3490 B	CA C	ALA B	46	-3.327	37.441	-9.309	1.00
25	ATOM 23.95	3491 B	CB C	ALA B	46	-4.271	37.895	-8.229	1.00
	ATOM 23.75	3492 B	C C	ALA B	46	-4.015	36.426	-10.216	1.00
30	ATOM 22.67	3493 B	0 0	ALA B	46	-4.777	36.788	-11.103	1.00
	ATOM 23.77	3494 B	N N	GLN B	47	-3.717	35.150	-9.982	1.00

	ATOM 24.59	3495 B	CA C	GLN	В	47	-4.438	34.035	-10.568	1.00
	ATOM 25.29	3496 B	CB C	GLN	В	47	-3.479	32.976	-11.105	1.00
5	ATOM 28.88	3497 B	CG C	GLN	В	47	-2.425	33.498	-12.080	1.00
	ATOM 35.56	3498 B	CD C	GLN	В	47	-3.025	33.975	-13.393	1.00
10	ATOM 40.01	3499 B	OE1 O	GLN	В	47	-3.624	33.176	-14.144	1.00
	ATOM 38.46		NE2 N	GLN	В	47	-2.869	35.278	-13.686	1.00
	ATOM 23.84	3501 B	C C	GLN	В	47	-5.298	33.425	-9.460	1.00
15	ATOM 24.12	3502 B	0 0	GLN	В	47	-4.786	32.790	-8.517	1.00
	ATOM 22.91	3503 B	N N	ILE	В	48	-6.597	33.644	-9.559	1.00
20	ATOM 23.01	3504 B		ILE	В	48	-7.502	33.329	-8.463	1.00
	ATOM 22.88	3505 <sub>.</sub> B		ILE	В	48	-8.486	34.462	-8.235	1.00
	ATOM 22.10	3506 B	CG1 C	ILE	В	48	-7.708	35.747	-7.988	1.00
25	ATOM 22.38	3507 B	CD1 C	ILE	В	48	-8.568	36.992	-7.917	1.00
	ATOM 21.57	3508 B	CG2 C	ILE	В	48	-9.391	34.161	-7.036	1.00
30	ATOM 23.69	3509 B	C C	ILE	В	48	-8.230	32.047	-8.746	1.00
	ATOM 23.31	3510 B	0 0	ILE	В	48	-8.685	31.820	-9.877	1.00

	ATOM 23.55	3511 B	N N	ILE B	49	-8.277	31.206	-7.716	1.00
	ATOM 24.95	3512 B	CA C	ILE B	49	-8.894	29.894	-7.746	1.00
5	ATOM 26.22	3513 B	CB C	ILE B	49	-7.803	28.812	-7.480	1.00
	ATOM 29.02	3514 B	CG1 C	ILE B	49	-6.723	28.868	-8.575	1.00
10	ATOM 29.18	3515 B	CD1 C	ILE B	49	-7.264	28.733	-9.982	1.00
	ATOM 28.74	3516 B	CG2 C	ILE B	49	-8.409	27.422	-7.364	1.00
	ATOM 23.74	3517 B	C C	ILE B	49	-9.903	29.851	-6.610	1.00
15	ATOM 24.09	3518 B	0 0	ILE B	49	-9.620	30.348	-5.511	1.00
	ATOM 22.75	3519 B	N N	VAL B	50	-11.045	29.224	-6.847	1.00
20	ATOM 22.00	3520 B	CA C	VAL B	50	-12.088	29.110	-5.838	1.00
	ATOM 21.55	3521 B	CB C	VAL B	50	-13.441	29.682	-6.364	1.00
	ATOM 22.01	3522 B	CG1 C	VAL B	50	-14.583	29.378	-5.388	1.00
25	ATOM 21.04	3523 B	CG2 C	VAL B	50	-13.338	31.190	-6.581	1.00
	ATOM 21.99	3524 B	C C	VAL B	50	-12.273	27.639	-5.439	1.00
30	ATOM 21.98	3525 B	0	VAL B	50	-12.375	26.780	-6.291	1.00
	ATOM 21.70	3526 B	N N	LEU B	51	-12.318	27.363	-4.141	1.00

	ATOM 22.26	3527 B	CA C	LEU B	51	-12.460	26.003	-3.643	1.00
	ATOM 22.70	3528 B		LEU B	51	-11.110	25.407	-3.219	1.00
5	ATOM 25.11	3529 B		LEU B	51	-10.067	25.113	-4.267	1.00
	ATOM 25.85	3530 B	CD1 C	LEU B	51	-8.762	24.764	-3.495	1.00
10	ATOM 27.79		CD2 C	LEU B	51	-10.513	23.968	-5.183	1.00
	ATOM 21.80	3532 B		LEU B	51	-13.312	25.997	-2.406	1.00
	ATOM 21.46	3533 B	0 0	LEU B	51	-13.289	26.962	-1.646	1.00
15	ATOM 21.76	3534 B	N N	PRO B	52	-14.006	24.886	-2.163	1.00
	ATOM 22.13	3535 B	CA C	PRO B	52	-14.750	24.709	-0.921	1.00
20	ATOM 23.06	3536 B		PRO B	52	-15.340	23.290	-1.071	1.00
	ATOM 22.20		CG C	PRO B	52	-15.389	23.059	-2.525	1.00
	ATOM 22.25	3538 B	CD C	PRO B	52	-14.145	23.724	-3.058	1.00
25	ATOM 22.83	3539 B	C C	PRO B	52	-13.836	24.809	0.290	1.00
	ATOM 22.05	3540 B	0 0	PRO B	52	-12.682	24.367	0.252	1.00
30	ATOM 23.43	3541 B	N N	VAL B	53	-14.340	25.400	1.365	1.00
	ATOM 23.96	3542 B	CA C	VAL B	53	-13.579	25.504	2.581	1.00

	ATOM 24.41	3543 B	CB C	VAL	В	53	-14.297	26.368	3.643	1.00
	ATOM 25.13	3544 B	CG1 C	VAL	В	53	-15.583	25.692	4.134	1.00
5	ATOM 25.93	3545 B		VAL	В	53	-13.360	26.671	4.805	1.00
	ATOM 24.12	3546 B	C C	VAL	В	53	-13.324	24.083	3.068	1.00
10	ATOM 24.69	3547 B	0 0	VAL	В	53	-14.153	23.193	2.859	1.00
	ATOM 22.87			GLY	В	54	-12.158	23.867	3.657	1.00
	ATOM 22.48	3549 B	CA C	GLY	В	54	-11.765	22.548	4.117	1.00
15	ATOM 21.22	3550 B	C C	GLY	В	54	-11.067	21.662	3.092	1.00
	ATOM 21.63	3551 B	0 0	GLY	В	54	-10.597	20.606	3.453	1.00
20	ATOM 20.24	3552 B	N N	THR	В	55	-10.977	22.091	1.837	1.00
	ATOM 19.46	3553 B	CA C	THR	В	55	-10.295	21.324	0.809	1.00
	ATOM 19.86	3554 B	CB C	THR	В	55	-10.469	22.006	-0.573	1.00
25	ATOM 22.41	3555 B	OG1 O	THR	В	55	-11.866	22.158	-0.875	1.00
	ATOM 19.94	3556 B	CG2 C	THR	В	55	-9.957	21.139	-1.701	1.00
30	ATOM 17.93	3557 B	C C	THR	В	55	-8.788	21.125	1.077	1.00
	ATOM 16.91	3558 B	0 0	THR	В	55	-8.057	22.042	1.417	1.00

	ATOM 17.04	3559 B	N N	ILE	В	56	-8.336	19.911	0.849	1.00
	ATOM 16.44	3560 B	CA C	ILE	В	56	-6.929	19.571	0.943	1.00
5	ATOM 15.71	3561 B		ILE	В	56	-6.800	18.076	1.232	1.00
	ATOM 17.41	3562 B	CG1 C	ILE	В	56	-7.439	17.782	2.600	1.00
10	ATOM 17.17		CD1 C	ILE	В	56	-7.353	16.319	3.098	1.00
	ATOM 16.77		CG2 C	ILE	В	56	-5.347	17.684	1.247	1.00
	ATOM 16.51	3565 B		ILE	В	56	-6.217	19.981	-0.336	1.00
15	ATOM 17.03	3566 B	0 0	ILE	В	56	-6.701	19.691	-1.434	1.00
	ATOM 15.94	3567 B	N N	VAL	В	57	-5.088	20.678	-0.203	1.00
20	ATOM 16.45	3568 B	CA C	VAL	В	57	-4.342	21.200	-1.361	1.00
	ATOM 16.21	3569 B	CB C	VAL	В	57	-4.511	22.726	-1.488	1.00
	ATOM 16.73	3570 B	CG1 C	VAL	В	57	-6.012	23.092	-1.672	1.00
25	ATOM 18.16	3571 B	CG2 C	VAL	В	57	-3.991	23.435	-0.236	1.00
	ATOM 16.63	3572 B	C C	VAL	В	57	-2.853	20.910	-1.205	1.00
30	ATOM 16.42	3573 B	0 0	VAL	В	57	-2.393	20.624	-0.099	1.00
	ATOM 17.06	3574 B	N N	THR	В	58	-2.106	20.982	-2.299	1.00

	ATOM 16.63	3575 B	CA C	THR	В	58	-0.658	20.801	-2.247	1.00
	ATOM 17.18	3576 B		THR	В	58	-0.069	20.712	-3.654	1.00
5	ATOM 15.16		OG1 O	THR	В	58	-0.660	21.718	-4.494	1.00
	ATOM 19.58	3578 B	CG2 C	THR	В	58	-0.423	19.426	-4.292	1.00
10	ATOM 16.72	3579 B	C C	THR	В	58	-0.093	22.017	-1.536	1.00
		3580 B		THR	В	58	-0.756	23.071	-1.492	1.00
	ATOM 16.38	3581 B	N N	MET	В	59	1.103	21.885	-0.960	1.00
15	ATOM 16.07	3582 B	CA C	MET	В	59	1.692	22.982	-0.180	1.00
	ATOM 15.92	3583 B	CB C	MET	В	59	1.960	22.552	1.254	1.00
20	ATOM 16.14		CG C	MET	В	59	0.668	22.365	2.012	1.00
	ATOM 17.09	3585 B		MET	В	59	-0.197	23.961	2.251	1.00
	ATOM 17.23	3586 B	CE C	MET	В	59	-1.612	23.424	3.218	1.00
25	ATOM 15.83	3587 B	C C	MET	В	59	2.911	23.607	-0.816	1.00
	ATOM 15.99	3588 B	0 0	MET	В	59	3.884	23.983	-0.134	1.00
30	ATOM 15.11	3589 B	N N	GLU	В	60	2.837	23.794	-2.127	1.00
	ATOM 15.22	3590 B	CA C	GLU	В	60	3.838	24.609	-2.795	1.00

	ATOM 15.39	3591 B	CB C	GLU	В	60	4.155	24.079	-4.187	1.00
	ATOM 15.29	3592 B	CG C	GLU	В	60	3.299	24.609	-5.334	1.00
5	ATOM 19.22	3593 B	CD C	GLU	В	60	1.845	24.166	-5.270	1.00
	ATOM 18.05	3594 B	OE1 O	GLU	В	60	1.435	23.486	-4.308	1.00
10	ATOM 18.12	3595 B	OE2 O	GLU	В	60	1.087	24.526	-6.195	1.00
	ATOM 15.50	3596 B	C C	GLU	В	60	3.344	26.081	-2.771	1.00
	ATOM 15.17	3597 B	0 0	GLU	В	60	2.133	26.356	-2.798	1.00
15	ATOM 16.00	3598 B	N N	TYR	В	61	4.292	27.011	-2.721	1.00
	ATOM 17.37	3599 B	CA C	TYR	В	61	3.982	28.431	-2.654	1.00
20	ATOM 17.67	3600 B	CB C	TYR	В	61	4.938	29.138	-1.699	1.00
	ATOM 18.81	3601 B	CG C	TYR	В	61	4.671	30.623	-1.493	1.00
	ATOM 21.63	3602 B	CD1 C	TYR	В	61	5.474	31.572	-2.103	1.00
25	ATOM 21.96	3603 B	CE1 C	TYR	В	61	5.233	32.895	-1.943	1.00
	ATOM 22.89	3604 B	CZ C	TYR	В	61	4.207	33.299	-1.134	1.00
30	ATOM 29.91	3605 B	OH	TYR	В	61	4.007	34.644	-0.972	1.00
	ATOM 20.81	3606 B	CE2 C	TYR	В	61	3.407	32.394	-0.507	1.00

	ATOM 19.36	3607 B	CD2 C	TYR	В	61	3.637	31.059	-0.697	1.00
	ATOM 18.22		C C	TYR	В	61	4.067	29.037	-4.048	1.00
5	ATOM 18.04	3609 B	0 0	TYR	В	61	5.126	29.041	-4.654	1.00
	ATOM 19.75	3610 B	N N	ARG	В	62	2.943	29.531	-4.564	1.00
10	ATOM 21.16			ARG	В	62	2.938	30.226	-5.861	1.00
	ATOM 21.92			ARG	В	62	1.909	29.625	-6.814	1.00
	ATOM 25.65	3613 B		ARG	В	62	2.189	28.185	-7.196	1.00
15	ATOM 29.39		CD C	ARG	В	62	1.385	27.694	-8.421	1.00
	ATOM 32.04	3615 B		ARG	В	62	1.516	26.235	-8.639	1.00
20	ATOM 33.94		CZ C	ARG	В	62	0.982	25.593	-9.675	1.00
	ATOM 37.42	_	NH1 N	ARG	В	62	1.129	24.287	-9.798	1.00
	ATOM 34.66	3618 B	NH2 N	ARG	В	62	0.292	26.255	-10.586	1.00
25	ATOM 21.86	3619 B	C C	ARG	В	62	2.619	31.687	-5.652	1.00
	ATOM 21.34	3620 B	0 0	ARG	В	62	1.491	32.033	-5.296	1.00
30	ATOM 23.01	3621 B	N N	ILE	В	63	3.609	32.547	-5.894	1.00
	ATOM 24.71	3622 B	CA C	ILE	В	63	3.503	33.950	-5.502	1.00

	ATOM 25.05	3623 B	CB ILE C	В	63	4.824	34.707	-5.709	1.00
	ATOM 28.83	3624 B	CG1 ILE C	В	63	4.790	36.033	-4.919	1.00
5	ATOM 31.61	3625 B	CD1 ILE C	В	63	6.158	36.609	-4.546	1.00
	ATOM 26.58		CG2 ILE	В	63	5.047	34.966	-7.207	1.00
10	ATOM 24.34		C ILE	В	63	2.367	34.699	-6.216	1.00
	ATOM 25.45		O ILE	В	63	1.860	35.675	-5.672	1.00
	ATOM 24.15	3629 B	N ASP	В	64	1.961	34.240	-7.398	1.00
15	ATOM 24.63	3630 B	CA ASP	В	64	0.901	34.919	-8.153	1.00
	ATOM 24.94	3631 B	CB BASP C	В	64	1.214	34.889	-9.664	0.40
20	ATOM 24.96		CB AASP C	В	64	1.201	34.873	-9.650	0.60
	ATOM 25.65	3633 B	CG BASP	В	64	0.987	33.514	-10.307	0.40
	ATOM 25.91	3634 B	CG AASP C	В	64	2.403	35.712	-10.026	0.60
25	ATOM 27.17	3635 B	OD1BASP O	В	64	0.745	33.465	-11.536	0.40
	ATOM 27.52	3636 B	OD1AASP O	В	64	3.136	35.290	-10.950	0.60
30	ATOM 28.49	3637 B		В	64	1.054	32.426	-9.686	0.40
	ATOM 26.67	3638 B	OD2AASP O	В	64	2.704	36.782	-9.439	0.60

	ATOM 24.47	3639 B	C C	ASP	В	64	-0.514	34.361	-7.896	1.00
	ATOM 24.83	3640 B	0 0	ASP	В	64	-1.515	34.928	-8.392	1.00
5	ATOM 21.92	3641 B	N N	ARG	В	65	-0.601	33.269	-7.136	1.00
	ATOM 21.12	3642 B	CA C	ARG	В	65	-1.876	32.615	-6.893	1.00
10	ATOM 19.95	3643 B	CB C	ARG	В	65	-1.677	31.101	-6.737	1.00
	ATOM 18.99	3644 B	CG C	ARG	В	65	-2.946	30.305	-6.463	1.00
	ATOM 19.09	3645 B	CD C	ARG	В	65	-2.730	28.808	-6.572	1.00
15	ATOM 18.66	3646 B	NE N	ARG	В	65	-1.784	28.369	-5.554	1.00
	ATOM 19.41	3647 B	CZ C	ARG	В	65	-1.130	27.214	-5.534	1.00
20	ATOM 19.74	3648 B	NH1 N	ARG	В	65	-1.279	26.300	-6.470	1.00
	ATOM 21.82	3649 B	NH2 N	ARG	В	65	-0.311	26.963	-4.522	1.00
	ATOM 20.36	3650 B	C C	ARG	В	65	-2.556	33.168	-5.662	1.00
25	ATOM 21.06	3651 B	0 0	ARG	В	65	-1.896	33.515	-4.682	1.00
	ATOM 20.04	3652 B	N N	VAL	В	66	-3.875	33.284	-5.727	1.00
30	ATOM 19.79	3653 B	CA C	VAL	В	66	-4.692	33.540	-4.560	1.00
	ATOM 19.88	3654 B	CB C	VAL	В	66	-5.266	34.962	-4.510	1.00

	ATOM 21.06	3655 B	CG1 C	VAL	В	66	-6.036	35.160	-3.204	1.00
	ATOM 20.96	3656 B	CG2 C	VAL	В	66	-4.194	36.004	-4.607	1.00
5	ATOM 20.19	3657 B	C C	VAL	В	66	-5.846	32.525	-4.551	1.00
	ATOM 20.12	3658 B	0 0	VAL	В	66	-6.733	32.512	-5.444	1.00
10	ATOM 20.01	3659 B		ARG	В	67	-5.832	31.654	-3.557	1.00
	ATOM 20.45		CA C	ARG	В	67	-6.916	30.713	-3.394	1.00
	ATOM 20.71	3661 B		ARG	В	67	-6.416	29.437	-2.740	1.00
15	ATOM 21.28	3662 B	CG C	ARG	В	67	-5.572	28.538	-3.626	1.00
	ATOM 23.63		CD C	ARG	В	67	-5.471	27.144	-3.016	1.00
20	ATOM 22.50	3664 B		ARG	В	67	-4.539	26.204	-3.632	1.00
	ATOM 24.19	3665 B		ARG	В	67	-3.326	25.921	-3.160	1.00
	ATOM 22.65	3666 B	NH1 N	ARG	B.	67	-2.589	24.992	-3.759	1.00
25	ATOM 22.06	3667 B	NH2 N	ARG	В	67	-2.837	26.571	-2.106	1.00
	ATOM 20.49	3668 B	C C	ARG	В	67	-8.001	31.368	-2.543	1.00
30	ATOM 20.17	3669 B	0 0	ARG	В	67	-7.704	31.990	-1.529	1.00
	ATOM 20.39	3670 B	N N	LEU	В	68	-9.255	31.253	-2.970	1.00

	ATOM 21.05	3671 B	CA C	LEU	В	68	-10.373	31.705	-2.148	1.00
	ATOM 21.11	3672 B	CB C	LEU	В	68	-11.323	32.604	-2.957	1.00
5	ATOM 21.59	3673 B	CG C	LEU	В	68	-10.701	33.830	-3.627	1.00
	ATOM 22.82	3674 B	CD1 C	LEU	В	68	-11.745	34.523	-4.508	1.00
10	ATOM 22.44	3675 B	CD2 C	LEU	В	68	-10.187	34.785	-2.595	1.00
	ATOM 21.12	3676 B	C C	LEU	В	68	-11.132	30.493	-1.648	1.00
	ATOM 21.87	3677 B	0 0	LEU	В	68	-11.663	29.709	-2.432	1.00
15	ATOM 21.61	3678 B	N N	PHE	В	69	-11.209	30.345	-0.345	1.00
	ATOM 21.97	3679 B	CA C	PHE	В	69	-11.937	29.226	0.233	1.00
20	ATOM 22.17	3680 B	CB C	PHE	В	69	-11.151	28.647	1.422	1.00
	ATOM 19.89	3681 B		PHE	В	69	-9.896	27.905	1.028	1.00
	ATOM 21.41	3682 B	CD1 C	PHE	В	69	-9.938	26.557	0.737	1.00
25	ATOM 20.29	3683 B	CE1 C	PHE	В	69	-8.788	25.862	0.370	1.00
	ATOM 21.78	3684 B	CZ C	PHE	В	69	-7.598	26.525	0.290	1.00
30	ATOM 21.52	3685 B	CE2 C	PHE	В	69	-7.542	27.879	0.575	1.00
	ATOM 19.33	3686 B	CD2 C	PHE	В	69	-8.691	28.557	0.950	1.00

	ATOM 23.11	3687 B	C C	PHE	В	69	-13.321	29.725	0.664	1.00
	ATOM 22.87		0 0	PHE	В	69	-13.414	30.651	1.506	1.00
5	ATOM 24.00	3689 B		VAL	В	70	-14.371	29.105	0.111	1.00
	ATOM 25.82	3690 B	CA C	VAL	В	70	-15.755	29.578	0.289	1.00
10	ATOM 25.72			VAL	В	70	-16.442	29.958	-1.054	1.00
	ATOM 26.70	3692 B	CG1 C	VAL	В	70	-15.686	31.063	-1.756	1.00
	ATOM 26.63	3693 B	CG2 C	VAL	В	70	-16.599	28.756	-1.958	1.00
15	ATOM 26.63		C C	VAL	В	70	-16.691	28.602	0.996	1.00
•		3695 B		VAL	В	70	-16.532	27.380	0.899	1.00
20	ATOM 27.52	3696 B		ASP	В	71	-17.664	29.155	1.714	1.00
	ATOM 29.00	3697 B		ASP	В	71	-18.686	28.352	2.399	1.00
	ATOM 28.91	3698 B	CB C	ASP	В	71	-19.247	29.132	3.591	1.00
25	ATOM 28.74	3699 B	CG C	ASP	В	71	-20.019	30.392	3.171	1.00
	ATOM 29.94	3700 B	OD1 O	ASP	В	71	-20.161	31.290	4.018	1.00
30	ATOM 27.69	3701 B	OD2 O	ASP	В	71	-20.509	30.572	2.032	1.00
	ATOM 30.37	3702 B	C C	ASP	В	71	-19.796	27.931	1.413	1.00

	ATOM 29.90	3703 B	0 0	ASP	В	71	-19.646	28.098	0.217	1.00
	ATOM 33.42	3704 B	N N	LYS	В	72	-20.898	27.376	1.906	1.00
5	ATOM 34.98	3705 B	CA C	LYS	В	72	-21.949	26.822	1.022	1.00
	ATOM 35.44	3706 B	CB C	LYS	В	72	-22.951	26.004	1.834	1.00
10	ATOM 40.00	3707 B	CG C	LYS	В	72	-22.190	24.925	2.916	0.00
	ATOM 40.00	3708 B	CD C	LYS	В	72	-22.489	23.435	2.595	0.00
	ATOM 40.00	3709 B		LYS	В	72	-21.240	22.528	2.667	0.00
15	ATOM 40.00	3710 B	NZ N	LYS	В	72	-21.120	21.662	1.456	0.00
	ATOM 36.38	3711 B	C C	LYS	В	72	-22.709	27.904	0.261	1.00
20	ATOM 37.77		0 0	LYS	В	72	-23.332	27.627	-0.766	1.00
	ATOM 37.07	3713 B	N N	LEU	В	73	-22.640	29.138	0.753	1.00
	ATOM 37.22	3714 B	CA C	LEU	В	73	-23.306	30.286	0.114	1.00
25	ATOM 37.50	3715 B	CB C	LEU	В	73	-23.759	31.265	1.201	1.00
	ATOM 40.20	3716 B	CG C	LEU	В	73	-24.711	30.678	2.254	1.00
30	ATOM 41.53	3717 B	CD1 C	LEU	В	73	-25.387	31.796	3.053	1.00
	ATOM 41.89	3718 B	CD2 C	LEU	В	73	-25.782	29.775	1.612	1.00

	ATOM 36.59	3719 B	C C	LEU	В	73	-22.406	31.008	-0.890	1.00
	ATOM 36.18	3720 B	0 0	LEU	В	73	-22.781	32.029	-1.482	1.00
5	ATOM 36.33	3721 B	N N	ASP	В	74	-21.203	30.468	-1.076	1.00
	ATOM 35.65	3722 B	CA C	ASP	В	74	-20.192	31.084	-1.923	1.00
10	ATOM 36.81	3723 B	CB C	ASP	В	74	-20.709	31.252	-3.342	1.00
		3724 B		ASP	В	74	-20.063	30.283	-4.286	1.00
	ATOM 45.75	3725 B		ASP	В	74	-19.429	30.756	-5.259	1.00
15	ATOM 45.61	3726 B	OD2 O	ASP	В	74	-20.108	29.032	-4.101	1.00
	ATOM 33.94	3727 B	C C	ASP	В	74	-19.646	32.399	-1.381	1.00
20	ATOM 34.59	3728 B	0 0	ASP	В	74	-19.147	33.249	-2.136	1.00
	ATOM 31.85		N N	ASN	В	75	-19.696	32.546	-0.066	1.00
	ATOM 30.66	3730 B	CA C	ASN	В	75	-19.000	33.634	0.597	1.00
25	ATOM 30.45	3731 B	CB C	ASN	В	75	-19.877	34.185	1.714	1.00
	ATOM 30.77	3732 B	CG C	ASN	В	75	-21.170	34.793	1.176	1.00
30	ATOM 30.57	3733 B	OD1 O	ASN	В	75	-21.169	35.401	0.102	1.00
	ATOM 30.32	3734 B	ND2 N	ASN	В	75	-22.275	34.615	1.907	1.00

	ATOM 29.26	3735 B	C C	ASN	В	75	-17.628	33.213	1.127	1.00
	ATOM 29.07	3736 B	0 0	ASN	В	75	-17.433	32.073	1.553	1.00
5	ATOM 27.83	3737 B	N N	ILE	В	76	-16.685	34.143	1.086	1.00
	ATOM 26.88	3738 B	CA C	ILE	В	76	-15.337	33.893	1.540	1.00
10	ATOM 26.51	3739 B		ILE	В	76	-14.511	35.182	1.455	1.00
			CG1 C	ILE	В	76	-14.474	35.737	0.020	1.00
	ATOM 26.87	3741 B		ILE	В	76	-14.130	34.728	-1.039	1.00
15	ATOM 25.62	3742 B	CG2 C	ILE	В	76	-13.137	34.927	1.993	1.00
	ATOM 26.59	3743 B	C C	ILE	В	76	-15.401	33.382	2.993	1.00
20	ATOM 26.12	3744 B	0 0	ILE	В	76	-15.994	34.017	3.838	1.00
	ATOM 26.58	3745 B		ALA	В	77	-14.795	32.237	3.263	1.00
	ATOM 26.79	3746 B	CA C	ALA	В	77	-14.899	31.582	4.576	1.00
25	ATOM 26.56	3747 B	CB C	ALA	В	77	-15.129	30.088	4.386	1.00
	ATOM 26.89	3748 B	C C	ALA	В	77	-13.670	31.815	5.467	1.00
30	ATOM 27.73	3749 B	0 0	ALA	В	77	-13.764	31.751	6.677	1.00
	ATOM 26.32	3750 B	N N	GLU	В	78	-12.518	32.072	4.871	1.00

	ATOM 26.33	3751 B	CA C	GLU	в 78	-11.355	32.446	5.647	1.00
	ATOM 26.80	3752 B	CB C	GLU	В 78	-10.508	31.216	6.041	1.00
5	ATOM 27.82	3753 B	CG C	GLU	В 78	-10.106	30.290	4.921	1.00
	ATOM 28.92	3754 B	CD C	GLU :	B 78	-9.956	28.827	5.352	1.00
10	ATOM 36.40	3755 B	OE1 O	GLU 1	B 78	-9.785	28.493	6.559	1.00
	ATOM 28.50	3756 B	OE2 O	GLU :	B 78	-10.001	27.977	4.472	1.00
	ATOM 25.94	3757 B	C C	GLU	В 78	-10.530	33.478	4.895	1.00
15	ATOM 25.71	3758 B	0	GLU	B 78	-10.807	33.805	3.712	1.00
	ATOM 24.85	3759 B	N N	VAL	B 79	-9.527	33.996	5.594	1.00
20	ATOM 24.88	3760 B	CA C	VAL	B 79	-8.712	35.088	5.102	1.00
	ATOM 25.77	3761 B	CB C	VAL	В 79	-7.692	35.578	6.167	1.00
	ATOM 25.38	3762 B	CG1 C	VAL 1	в 79	-6.814	36.672	5.583	1.00
25	ATOM 26.10	3763 B	CG2 C	VAL 1	в 79	-8.396	36.073	7.456	1.00
	ATOM 24.07	3764 B	C C	VAL	B 79	-7.957	34.652	3.835	1.00
30	ATOM 23.32	3765 B	0 0	VAL	В 79	-7.137	33.742	3.883	1.00
	ATOM 23.27	3766 B	N N	PRO	B 80	-8.275	35.271	2.699	1.00

	ATOM 22.93	3767 B	CA PRO B	80	-7.533	35.029	1.466	1.00
	ATOM 23.15	3768 B	CB PRO B	80	-8.296	35.856	0.426	1.00
5	ATOM 23.83	3769 B	CG PRO B	80	-9.645	36.042	1.005	1.00
	ATOM 23.67	3770 B	CD PRO B	80	-9.404	36.194	2.480	1.00
10	ATOM 22.05	3771 B	C PRO B	80	-6.101	35.512	1.601	1.00
	ATOM 20.76	3772 B	O PRO B	80	-5.891	36.588	2.136	1.00
	ATOM 21.54	3773 B	N ARG B	81	-5.147	34.691	1.190	1.00
15	ATOM 22.93	3774 B	CA ARG B	81	-3.765	35.135	1.074	1.00
	ATOM 22.99	3775 B	CB BARG B	81	-2.937	34.683	2.298	0.40
20	ATOM 23.27	3776 B	CB AARG B	81	-2.865	34.764	2.275	0.60
	ATOM 24.27	3777 B	CG BARG B	81	-3.684	34.672	3.645	0.40
	ATOM 25.79	3778 B	CG AARG B C	81	-3.278	33.619	3.175	0.60
25	ATOM 26.79	3779 B	CD BARG B	81	-2.996	33.818	4.744	0.40
	ATOM 27.67	3780 B	CD AARG B	81	-2.615	33.723	4.575	0.60
30	ATOM 28.96	3781 B	NE BARG B	81	-3.975	33.234	5.664	0.40
	ATOM 29.38	3782 B	NE AARG B	81	-3.283	32.907	5.581	0.60

	ATOM 29.28	3783 B	CZ BARG B	81	-4.567	32.053	5.508	0.40
	ATOM 30.17	3784 B	CZ AARG B C	81	-3.934	33.381	6.642	0.60
5	ATOM 31.06	3785 B	NH1BARG B N	81	-4.284	31.274	4.471	0.40
	ATOM 3786 NH1AARG 31.08 B N			81	-4.020	34.680	6.867	0.60
10	ATOM 30.62	3787 B	NH2BARG B N	81	-5.448	31.645	6.408	0.40
	ATOM 31.16	3788 B	NH2AARG B N	81	-4.510	32.545	7.486	0.60
	ATOM 21.97	3789 B	C ARG B	81	-3.115	34.616	-0.178	1.00
15	ATOM 21.68	3790 B	O ARG B	81	-3.560	33.632	-0.761	1.00
	ATOM 20.91	3791 B	N VAL B	82	-2.029	35.286	-0.559	1.00
20	ATOM 21.03	3792 B	CA VAL B	82	-1.224	34.884	-1.679	1.00
	ATOM 21.89	3793 B	CB VAL B	82	-0.126	35.943	-1.952	1.00
	ATOM 22.93	3794 B	CG1 VAL B	82	0.869	35.435	-2.906	1.00
25	ATOM 21.44	3795 B	CG2 VAL B	82	-0.734	37.243	-2.483	1.00
	ATOM 20.69	3796 B	C VAL B	82	-0.583	33.532	-1.371	1.00
30	ATOM 19.36	3797 B	O VAL B	82	-0.235	33.255	-0.221	1.00
	ATOM 19.91	3798 B	N GLY B	83	-0.469	32.694	-2.389	1.00

	ATOM 20.16	3799 B	CA C	GLY	В	83	0.382	31.525	-2.331	1.00
	ATOM 20.11	3800 B	C C	GLY	В	83	-0.236	30.295	-2.955	1.00
5	ATOM 20.36	3801 B	0 0	GLY	В	83	-1.416	30.328	-3.319	1.00
	ATOM 18.79	3802 B	OXT O	GLY	В	83	0.468	29.294	-3.104	1.00